Exactly Solvable Models for Atom-Molecule Hamiltonians

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(Received 3 December 2003; published 30 July 2004)

We present a family of exactly solvable generalizations of the Jaynes-Cummings model involving the interaction of an ensemble of SU(2) or SU(1, 1) quasispins with a single boson field. They are obtained from the trigonometric Richardson-Gaudin models by replacing one of the SU(2) or SU(1, 1) degrees of freedom by an ideal boson. The application to a system of bosonic atoms and molecules is reported.

DOI: 10.1103/PhysRevLett.93.050403 PACS numbers: 03.75.–b, 02.30.Ik, 05.30.–d, 42.50.Pq

The Jaynes-Cummings (JC) model [1] provides a simple description of the interaction of matter with a radiation field. It treats a two-level atom in terms of the spin-1/2 generators of the SU(2) algebra and describes its coupling to a single radiation field in the so-called rotating wave approximation. Despite its simplicity, the model has had enormous success in quantum optics, finding realization in experiments with Rydberg atoms in microwave cavities [2] and optical cavities [3].

There have also been several extensions of the JC model that have likewise proven useful. One example is the Tavis-Cummings model [4], in which the spin-1/2 operators are replaced by operators for arbitrary spin, permitting the description of a collection of equivalent two-level atoms in a radiation field. This model has been solved exactly using the quantum inverse scattering method [5]. Another example is the Buck-Sukumar (BS) model [6], in which a specific nonlinear interaction between the atoms and the radiation field is included and which is also exactly solvable. The BS model is an example of a general class of models in which the radiation field is represented by an SU(1, 1) algebra and which are also exactly solvable [7]. More general nonlinear terms have also been discussed, but they can be treated only approximately [8]. A third example is an exactly solvable atom-molecule Hamiltonian that describes the photoassociation of pairs of condensed bosonic atoms—based on the algebra SU(1, 1), rather than SU(2)—into molecules with a linear interaction [9] or with a nonlinear interaction [7].

Similar physics is also at play when a molecular Bose-Einstein condensate (BEC) is produced through photoassociation (with or without the interaction with a Feshbach resonance) in dilute fermion [10] or boson [11] gases. The production of degenerate bosonic sodium atom-molecule mixtures has been recently reported [12], though it is still an open question as to whether the molecules formed a BEC. Mixtures of fermion atoms and molecular dimers are better candidates for constructing a molecular BEC due to the suppression of molecular decay by Pauli blocking. Indeed, two groups have reported the manufacture of molecular BECs from ^{40}K [13] and ^{6}Li [14] fermionic atoms, respectively. Unfortunately, no current exactly solvable model can describe these physical processes.

In this Letter, we show how to generalize the JC model to accommodate these physical scenarios, as well as others, in the context of exactly solvable models. The extension is to a family of models that involve an ensemble of SU(2) or SU(1, 1) quasispins and a single bosonic mode. For the purposes of our discussion, the SU(2) models describe fermion pairs and their coupling to a bosonic mode, whereas the SU(1, 1) models describe the corresponding physics of bosonic pairs. The SU(2) models could also be used to describe two-level atoms and a bosonic mode, but we do not discuss such models here. The generalizations we describe build on the recently proposed Richardson-Gaudin (RG) integrable models [15] (for a recent review see [16]). Following the presentation of the models, we discuss their specific application to a mixture of bosonic atoms and molecular dimers.

We begin by introducing the generators of the SU(2) and SU(1, 1) algebras, K_i^0, K_i^+, and $K_i^- = (K_i^+)^\dagger$, which satisfy the commutation relations

$$[K_i^0, K_j^+] = \delta_{ij} K_i^+, \qquad [K_i^+, K_j^-] = \mp 2\delta_{ij} K_i^0. \tag{1}$$

The upper sign refers to the bosonic SU(1, 1) algebra and the lower sign to the fermionic SU(2) algebra, as they do throughout this presentation.

In the quasispin or pair representation of the SU(2) and SU(1, 1) algebras, the generators are realized in terms of particle creation and annihilation operators as

$$K_j^0 = \frac{1}{2}\sum_m a_{jm}^\dagger a_{jm} \pm \frac{\Omega_j}{4}, \qquad K_j^+ = \frac{1}{2}\sum_m a_{jm}^\dagger a_{j\bar{m}}^\dagger. \tag{2}$$

Here $a_{jm}^\dagger$ (a_{jm}) creates (annihilates) a boson or a fermion in the state $|jm\rangle$, $|j\bar{m}\rangle$ is the state obtained by acting with the time reversal operator on $|jm\rangle$, and Ω_j is the total degeneracy of single-particle level j.

 0031-9007/04/93(5)/050403(4)$22.50

There are three families of fully integrable and exactly solvable RG models that derive from the SU(2) and SU(1, 1) algebras, the rational, trigonometric, and hyperbolic families, respectively [15]. For all three, it has been shown how to write the complete set of commuting integrals of motion and the corresponding eigenvalues and eigenvectors. Here we focus on the trigonometric family, for which they can be expressed in terms of the generators as

$$R_i = K_i^0 + 2g \sum_{j(\neq i)} \left\{ \frac{1}{2\sin(\eta_i - \eta_j)} [K_i^+ K_j^- + K_i^- K_j^+] \mp \cot(\eta_i - \eta_j) K_i^0 K_j^0 \right\}. \quad (3)$$

For each degree of freedom i, there is one real arbitrary parameter η_i that enters the integrals of motion.

We now consider the eigenvalue equation for the integrals of motion, $R_i|\Psi\rangle = r_i|\Psi\rangle$, in the seniority-zero sector, namely, when all particles are paired. Solutions with broken pairs can also be readily obtained, as in [15].

In this sector, the eigenstates of R_i are given by

$$|\Psi\rangle = \prod_{\alpha=1}^{M} B_\alpha^\dagger |0\rangle, \qquad B_\alpha^\dagger = \sum_l \frac{1}{\sin(e_\alpha - \eta_l)} K_l^+, \quad (4)$$

where $|0\rangle$ is a state that is annihilated by all the K_i^- and M is the number of pairs. The structure of the collective operators $B_\alpha^\dagger$ is determined by a set of M parameters e_α, which satisfy the set of coupled nonlinear equations

$$1 - \frac{g}{2} \sum_j \Omega_j \cot(e_\alpha - \eta_j) \pm 2g \sum_{\beta(\neq\alpha)} \cot(e_\beta - e_\alpha) = 0. \quad (5)$$

The associated eigenvalues take the form

$$r_i = \pm \frac{\Omega_i}{4} \left\{ 1 - \frac{g}{2} \sum_{j(\neq i)} \Omega_j \cot(\eta_i - \eta_j) \pm 2g \sum_\alpha \cot(e_\alpha - \eta_i) \right\}. \quad (6)$$

The important point to note here is that any Hamiltonian that can be written solely in terms of the integrals of motion R_i is likewise exactly solvable, with precisely the same eigenvectors as in (4) and with eigenvalues that are obtained directly from those in (6).

We now discuss how to construct from the trigonometric RG models a new class of exactly solvable models that involve the interplay of a set of SU(2) or SU(1, 1) systems with a single bosonic mode. To do this, we use a trick proposed by Gaudin [17], which involves replacing one SU(2) or SU(1, 1) degree of freedom by an ideal boson. For specificity, we denote the SU(2) or SU(1, 1) degree of freedom to be bosonized as $i = 0$ and the remaining as $i = 1, \ldots, L$. In the limit $\Omega_0 \to \infty$, the generators map onto ideal bosons according to

$$K_0^0 = b^\dagger b \pm \frac{\Omega_0}{4}, \qquad K_0^+ = \sqrt{\frac{\Omega_0}{2}}\, b^\dagger. \quad (7)$$

We now introduce a change of notation for the trigonometric functions that appear in (3) for the selected degree of freedom, $w_j = 1/\sin(\eta_0 - \eta_j)$, $v_j = \cot(\eta_0 - \eta_j)$, with $w_l^2 - v_l^2 = 1$. Moreover, we expand these amplitudes in the inverse of the divergent degeneracy Ω_0, $w_l^2 = 1 + \frac{2\varepsilon_l^2}{\Omega_0}$, $v_l = -\sqrt{\frac{2}{\Omega_0}}\,\varepsilon_l$, thereby introducing a new set of parameters ε_l ($l = 1, \ldots, L$) to replace the η_l's.

Inserting (7) and this new parametrization into (3), we obtain new integrals of motion that involve the ideal boson degree of freedom,

$$R_0 = b^\dagger b + G\left[\sum_j (b^\dagger K_j^- + K_j^+ b) + \sum_j \varepsilon_j K_j^0 \right], \quad (8)$$

$$R_j = K_j^0 + G\left[\sum_{i(\neq j)} \left\{ \frac{1}{(\varepsilon_i - \varepsilon_j)} [K_i^+ K_j^- + K_i^- K_j^+] \mp \frac{2}{\varepsilon_i - \varepsilon_j} K_i^0 K_j^0 \right\} - (K_j^+ b + K_j^- b^+) - \varepsilon_j K_j^0 \right], \quad (9)$$

where $G = g\sqrt{\Omega_0/2}$.

The resulting R_i still satisfy the conditions for an integrable model. They remain Hermitian, global, and independent, and mutually commute with one another, thereby constituting a complete set of integrals of motion. Thus, any Hamiltonian that can be written in terms of them likewise defines an exactly solvable model.

It is important to note that the integrals of motion in Eqs. (8) and (9) define *a totally new set of exactly solvable models*, even though they were derived from the trigonometric family of RG models. That they are not simply the trigonometric family rewritten can be seen by focusing on Eq. (9), which gives the form of the new R_j integrals of motion. They are, in fact, identical to those of the rational family of exactly solvable models, *except for the last two terms,* which are essential for ensuring commutation with the new bosonic integral of motion R_0.

Note further that the operator that counts the *total* number of pairs, $M = b^\dagger b + \frac{1}{2}\sum_{jm} a_{jm}^\dagger a_{jm}$, also commutes with all R_i and thus defines a conserved quantity.

Before continuing our derivation of the exact solutions associated with these integrals of motion, we first write down a particularly interesting Hamiltonian that can be treated exactly in this way. It is obtained directly from the selected integral of motion R_0,

$$H = \omega R_0 \mp \frac{\omega G}{4} \sum_j \Omega_j \varepsilon_j = \omega b^\dagger b + \sum_{jm} \epsilon_j a_{jm}^\dagger a_{jm} + V \sum_j (b^\dagger K_j^- + K_j^+ b), \quad (10)$$

where $V = \omega g\sqrt{\Omega_0/2}$ and $\epsilon_j = V\varepsilon_j/2$. In the pair representation of SU(2) or SU(1, 1), this Hamiltonian describes the interaction of fermionic or bosonic atom pairs with a diatomic molecule. In the two-level representation, it generalizes the Tavis-Cummings model to multiatoms.

Many other exactly solvable Hamiltonians can be derived by taking linear combinations of the other integrals of motion. This will lead, e.g., to Hamiltonians involving atom-atom pairing interactions and level-dependent atom-molecule couplings.

We now discuss how to rewrite the seniority-zero solutions for the trigonometric RG models to apply when one of its degrees of freedom has been replaced by an ideal boson in the infinite–Ω_0 limit. Defining $x_\alpha = \sqrt{\Omega_0/2}\cot(e_\alpha - \eta_0)$, the Richardson-Gaudin equations (5) that define the parameters e_α, and thus the x_α, become

$$\frac{1}{2G} - \frac{1}{2}x_\alpha - \frac{1}{4}\sum_j \frac{\Omega_j}{\varepsilon_j - x_\alpha} \mp \sum_{\beta(\neq\alpha)} \frac{1}{x_\beta - x_\alpha} = 0. \quad (11)$$

The corresponding expressions for the eigenvalues (6) associated with the new integrals of motion (8) and (9) are

$$r_0 = \pm\frac{G}{4}\sum_j \Omega_j\varepsilon_j + G\sum_\alpha x_\alpha, \quad (12)$$

$$r_i = \pm\frac{\Omega_i}{4} \times\left\{1 \mp 2G\left[\frac{1}{2}\varepsilon_i \pm \frac{1}{4}\sum_{j(\neq i)} \frac{\Omega_j}{\varepsilon_i - \varepsilon_j} + \sum_\alpha \frac{1}{x_\alpha - \varepsilon_i}\right]\right\}, \quad (13)$$

while the seniority-zero eigenvectors take the form

$$|\Psi\rangle = \prod_{\alpha=1}^{M}\left(b^\dagger + \sum_l \frac{1}{x_\alpha - \varepsilon_l}K_l^+\right)|0\rangle. \quad (14)$$

We note here that each independent solution of the set of nonlinear coupled Eqs. (11) defines an eigenstate (14) that is common to the $L + 1$ integrals of motion (8) and (9) and has eigenvalues (12) and (13).

The eigenvalues of the Hamiltonian (10), for example, can be obtained from the eigenvalues (12) of r_0 as

$$E = V\sum_\alpha x_\alpha. \quad (15)$$

It is worth noting here that the solutions given in (11)–(14) are identical to those of the Tavis-Cummings model [5] for a single SU(2) spin and to those for the atom-molecule model of [9] for a single SU(1, 1) bosonic level.

Important observables in these models are the occupation probabilities of the various degrees of freedom. They can be obtained from the integrals of motion using the Hellman-Feynman theorem, viz.,

$$\langle K_i^0\rangle = \langle R_i\rangle - G\left\langle\frac{\partial R_i}{\partial G}\right\rangle = r_i - G\frac{\partial r_i}{\partial G}, \quad (16)$$

from which we obtain for the occupation numbers

$$n_i = -\Omega_i G^2\sum_\alpha \frac{1}{(x_\alpha - \varepsilon_i)^2}\frac{\partial x_\alpha}{\partial G}. \quad (17)$$

The derivatives of the x_α are obtained by differentiating the RG Eqs. (11) with respect to G, which gives

$$\left[\pm\frac{1}{2} \pm \frac{1}{4}\sum_j \frac{\Omega_j}{(x_\alpha - \varepsilon_j)^2} + \sum_{\beta(\neq\alpha)} \frac{1}{(x_\beta - x_\alpha)^2}\right]\frac{\partial x_\alpha}{\partial G} - \sum_{\beta(\neq\alpha)} \frac{1}{(x_\beta - x_\alpha)^2}\frac{\partial x_\beta}{\partial G} = \mp\frac{1}{2G^2}. \quad (18)$$

We now describe a first application of these ideas, to demonstrate the feasibility of getting exact solutions for these models even for very large numbers of particles. We consider a mixture of bosonic atoms confined to a 3D isotropic trap coupled to a molecular two-particle bound state, a molecular dimer, and model it through the Hamiltonian (10). This Hamiltonian does not contain an atom-atom interaction, which could be included by using Hamiltonians derived from the other R_j's (9). In the Hamiltonian we use, ω is the energy of the molecular dimer above that of the Feshbach resonance and is the negative of the detuning parameter. Also, V is the atom-molecule interaction strength, $\epsilon_j = j$ $(j = 0, 1, \ldots)$ are the single-atom energies in a 3D isotropic trap, and $\Omega_j = (j + 1)(j + 2)/2$ are the level degeneracies. The phase diagram and dynamics of this model have been studied in several recent works, e.g., [18]. To make contact with Ref. [18], our detuning parameter is related to theirs by $\omega = \delta$ and our atom-molecule coupling is $V = -K/(2\sqrt{M})$.

As noted before, the complete set of seniority-zero eigenstates arises from different solutions of Eq. (11). For bosonic atoms, the parameters x_α are always real.

We have performed calculations for a system with $M = 500$ pairs and two values of the molecular energy, $\omega = 10$ and $\omega = -10$, as a function of the negative coupling V. The atom space was truncated to $L = 50$ harmonic oscillator shells. In Fig. 1, we show the occupation probabilities of the atomic condensate (solid line) and the atomic depletion (dashed line), and the fraction of molecules (dotted line) as a function of V for positive molecular energy ($\omega = 10$). As can be seen, a quantum phase transition takes place at $V \simeq -0.45$. Interestingly, the occupation of the atom condensed state is negligible for $V < -0.45$ and the atomic fraction is distributed among all harmonic oscillator levels. A pure molecular state does not exist for any value of V. This quantum phase transition was recently studied using mean-field and renormalization group techniques, and it was concluded

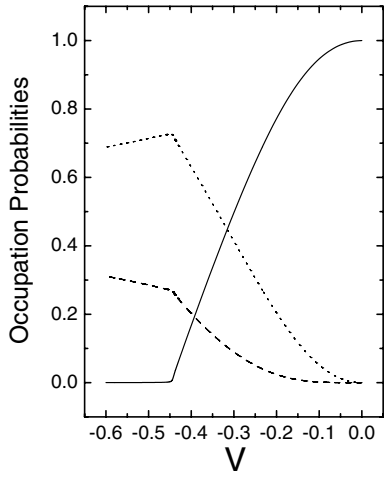

FIG. 1. Occupation probabilities as a function of the interaction V for a molecule energy $\omega = 10$. The solid line corresponds to condensed atoms, the dashed line to noncondensed atoms, and the dotted line to condensed molecules.

that it lies in the Ising universality class [19]. The exact solution offers a unique tool for exploring the critical properties around the transition point.

In Fig. 2 we show results for negative molecular energy, $\omega = -10$. The system is purely molecular for weak coupling. Molecules begin to decay to pair atomic states, as the interaction strengthens, but there is no phase transition and the occupation of the lowest trap level is always negligible. A detailed study of the phase diagram that emerges from the exact solutions will be given elsewhere.

In closing, we have presented in this Letter a new family of integrable models for atom-molecule systems. The models are exactly solvable for fermionic and bosonic atoms interacting with molecular dimers. There is a large freedom to select the parameters of the Hamiltonian, allowing for the description of quite general realistic systems. We presented initial results for a mixed system of trapped bosonic atoms and molecular dimers. Application to systems of fermionic atoms and molecular dimers is of special interest due to the recent generation of ultracold molecular BECs from the conversion of ^{40}K [13] and ^{6}Li [14] fermionic atoms. Such models can also be used to explore the BCS to BEC crossover, from a condensate dominated by Cooper pairs to one dominated by molecular dimers. Finally, it is possible to use alternative realizations of these models to describe problems of importance in quantum optics and perhaps elsewhere.

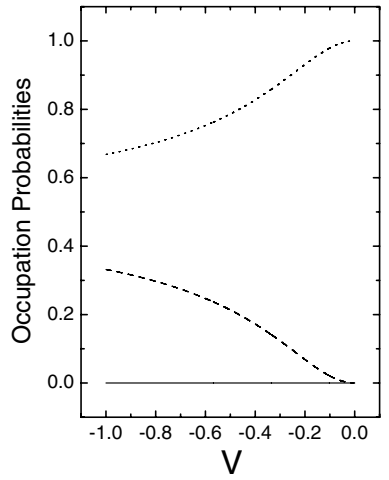

FIG. 2. Occupation probabilities as a function of the interaction V for a molecule energy $\omega = -10$. The solid line corresponds to condensed atoms, the dashed line to noncondensed atoms, and the dotted line to condensed molecules.

This work was supported by the Spanish DGI under Grant No. BFM2003-05316-C02-02, by the U.S. National Science Foundation under Grant No. PHY-0140036, and by UBACYT X-204. Fruitful discussions with L. L. Sanchez-Soto are acknowledged.

Note added.—After submitting this work, we learned of a recent paper on generalized integrable matter-radiation models [20]. The extended Jaynes-Cummings Hamiltonians treated therein have non-Hermitian atomic interactions.

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