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Many-body problems with composite particles and q-Heisenberg algebras

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Abstract. We propose to employ deformed commutation relations to treat many-body problems of composite particles. The deformation parameter is interpreted as a measure of the effects of the statistics of the internal degrees of freedom of the composite particles. A simple application of the method is made for the case of a gas of composite bosons.

In recent years there has been much interest in the subject of deformations of the basic commutation relations of Fermi and Bose fields. One focus of interest is on possible (small) violations of the Fermi and Bose statistics by particles ('quons') with annihilation and creation operators that obey deformed commutation relations which interpolate between bosons and fermions [1]. Another focus of interest closely related, not only in physics but also in mathematics, is the subject of quantum algebras [2], the origins of which are in the study of the Yang–Baxter equations connected with the quantum inverse scattering problem. The discovery by Macfarlane [3] and Biedenharm [4] of a new realization of the quantum algebra $su(2)_q$ in terms of q-analogues of the harmonic oscillator has given rise to speculations on possible applications in real physical problems. In addition to speculations on small violations of Fermi or Bose statistics [1] and on possible generalizations of quantum mechanics at higher energies (e.g. in the early universe) [5], quantum algebras have been used with relative success in phenomenological studies of deformed nuclei [6], diatomic molecules [7], spin chains [8] and anyonic oscillations with fractional statistics [9]. Despite successful phenomenological applications, a clear physical meaning of the deformation parameter q is lacking.

In this paper we propose employing a q-Heisenberg algebra [10] as a convenient tool to describe many-body problems involving composite particles (i.e. not point-like). We argue that the physical meaning of the deformation parameter is that it is a measure of the effects of the statistics of the internal degrees of freedom of the composite particles, and its value depends on the 'degree of overlap' of the extended structure of the particles in the medium. The interpretation that deformed algebras describe composite particles is not new and can be found in several places in the literature (see e.g. [1]); here we explicitly demonstrate the realization of this in a simple example. Many-body problems involving composite particles have complications in addition to the usual ones involving point particles due to the simultaneous presence of 'macroscopic' (composites) and 'microscopic' (constituents) degrees of freedom. Due to the internal degrees of freedom, the algebra of the creation and annihilation operators of the composite particles deviates from the usual canonical ones for point particles; it becomes deformed. It is therefore natural to speculate on the possibility that the deformation of the algebra of the creation and annihilation operators would provide a convenient way to take the microscopic degrees of freedom of the composites into account effectively. The deformation of the algebra is the price one pays for not taking the microscopic degrees of freedom explicitly into account. One can hope for the success of such a program for systems where the degree of overlap of the internal structures of the particles is not very large, in the sense that the system is not dissolved into its constituents. A related work [11] describes the possibility of using deformed commutation relations to treat correlated fermion pairs in a single-j nuclear shell.

We start with a heuristic discussion on the relation of the deformation parameter with the composite nature of bosons. We consider a composite boson state with quantum number α as a bound state of two distinct fermions:

$$A^\dagger_\alpha|0\rangle = \sum_{\mu\nu} \Phi^{\mu\nu}_\alpha a^\dagger_\mu b^\dagger_\nu |0\rangle \tag{1}$$

where $\Phi^{\mu\nu}_\alpha$ is the bound-state wavefunction, $a^\dagger_\mu$ and $b^\dagger_\mu$ are the fermion creation operators, and $|0\rangle$ is the vacuum state. The quantum number α stands for the centre-of-mass momentum, the internal energy, the spin and other internal degrees of freedom of the composite boson. The μ and ν stand for the space and internal quantum numbers of the constituent fermions. The sum over μ and ν is to be understood as a sum over discrete quantum numbers and an integral over continuous variables.

The fermion creation and annihilation operators satisfy canonical anticommutation relations:

$$\begin{aligned} &\{a_\mu, a_\nu\} = \{a^\dagger_\mu, a^\dagger_\nu\} = 0 \qquad \{b_\mu, b_\nu\} = \{b^\dagger_\mu, b^\dagger_\nu\} = 0 \\ &\{a_\mu, a^\dagger_\nu\} = \delta_{\mu,\nu} \qquad \{b_\mu, b^\dagger_\nu\} = \delta_{\mu,\nu}. \end{aligned} \tag{2}$$

It is convenient to work with normalized wavefunctions $\Phi^{\mu\nu}_\alpha$, such that

$$\langle\alpha|\beta\rangle = \delta_{\alpha,\beta} \tag{3}$$

and therefore

$$\sum_{\mu\nu} \Phi^{\mu\nu *}_\alpha \Phi^{\mu\nu}_\beta = \delta_{\alpha,\beta}. \tag{4}$$

Using the fermion anticommutation relations of equation (2) and the wavefunction normalization equation (4), one can easily show that the composite boson operators satisfy the following commutation relations:

$$[A_\alpha, A_\beta] = [A^\dagger_\alpha, A^\dagger_\beta] = 0 \qquad [A_\alpha, A^\dagger_\beta] = \delta_{\alpha,\beta} - \Delta_{\alpha\beta} \tag{5}$$

where $\Delta_{\alpha\beta}$ is given by

$$\Delta_{\alpha\beta} = \sum_{\mu\nu} \Phi^{\mu\nu *}_\alpha \left(\sum_{\mu'} \Phi^{\mu'\nu}_\beta a^\dagger_{\mu'} a_\mu + \sum_{\nu'} \Phi^{\mu\nu'}_\beta b^\dagger_{\nu'} b_\nu \right). \tag{6}$$

One can also easily show the following commutation relations:

$$\left[a_\mu, A^\dagger_\alpha\right] = \sum_{\mu'\nu'} \delta_{\mu,\mu'} \Phi^{\mu'\nu'}_\alpha b^\dagger_{\nu'} \qquad \left[b_\nu, A^\dagger_\alpha\right] = -\sum_{\mu'\nu'} \delta_{\nu,\nu'} \Phi^{\mu'\nu'}_\alpha a^\dagger_{\mu'}. \tag{7}$$

The composite nature of the bosons is evident from the presence of $\Delta_{\alpha\beta}$, it is a sort of a 'deformation' of the canonical boson algebra. The effect of this term becomes unimportant in the infinite tight binding limit, i.e. in the limit of point-like bosons. Equation (7) shows the lack of kinematical independence of the microscopic operators a_μ and b_ν from the macroscopic ones A'_αs.

Now let us consider a system of N composite bosons in a box of volume V at zero temperature. If the bosons were ideal point-like particles, the ground state of the system would be the one where all bosons condense in the zero momentum state. In the case of composite bosons, the closest analogue of the ideal-gas ground state is

$$|N\rangle = \frac{1}{\sqrt{N!}}(A_0^\dagger)^N|0\rangle \tag{8}$$

where $A_0^\dagger$ is the creation operator of a composite boson in its ground state (ground state Φ) and with zero centre-of-mass momentum. Due to the composite nature of the bosons, this state incorporates kinematical correlations implied by the Pauli exclusion principle which operates on the constituent fermions. Among other effects, the Pauli principle forbids the macroscopic occupation of the zero momentum state. The closest analogue to the boson occupation number in the state (8) is

$$N_0 = \frac{\langle N|A_0^\dagger A_0|N\rangle}{\langle N|N\rangle}. \tag{9}$$

In order to evaluate (9), we consider a spin-zero boson and use for the spatial part of Φ a simple Gaussian form such that the RMS radius of the boson is r_0. To lowest order in the density of the system $n = N/V$, N_0 is given by

$$N_0 = N\left(1 - \gamma n r_0^3\right) \tag{10}$$

where $\gamma = 4\pi^{-3/2} \simeq 1$ is a numerical factor that comes from the functional form of the wavefunction. If we had taken another functional form for Φ, we still would have obtained for N_0 the result of equation (10), but γ would have taken a different value.

It is apparent from equation (10) that in the limit of infinite tight binding, $r_0 \to 0$, one has the familiar Bose–Einstein condensation. For finite values for the size of the bosons, the effects of the Pauli principle become important and the amount of condensed bosons is depleted. Moreover, from (10) one has that if the size of the bound state is of the order of the mean separation of the bosons in the medium, $d \sim n^{-1/3}$, the depletion is almost total. The depletion of the condensation is a direct consequence of the deformation of the boson algebra by the term $\Delta_{\alpha\beta}$.

Next we show that the effect of the composite nature of the boson can effectively be taken into account by employing a deformed boson algebra. The deformed boson commutation relations are given by

$$A_\alpha A_\beta^\dagger - q^2 A_\beta^\dagger A_\alpha = \delta_{\alpha,\beta} \tag{11}$$

where q^2 is the deformation parameter of the algebra; A_α annihilates the vacuum

$$A_\alpha|0\rangle = 0. \tag{12}$$

Note that no commutation relation can be imposed on $A_\alpha^\dagger A_\alpha^\dagger$ and $A_\alpha A_\alpha$. However, as remarked by Greenberg [1], similarly to the case of normal Bose commutation relations, no such rule is needed for practical evaluation of expectation values of polynomials in A_α and $A_\alpha^\dagger$ when (12) holds. Such matrix elements can be evaluated with the repeated use of equation (11) solely; annihilation operators are moved to the right using (11) until they annihilate the vacuum or creation operators are moved to the left using the adjoint of (11) until they annihilate the vacuum.

If one writes $q^2 = 1 - x$, the deformed commutator can be written as

$$[A_\alpha, A_\beta^\dagger] = \delta_{\alpha,\beta} - xA_\alpha^\dagger A_\beta. \tag{13}$$

The similarity of this with the second equation of (5) is evident. In some sense, the weighted (by the Φ's) fermion operators $a_{\mu'}^\dagger a_\mu$ and $b_\mu^\dagger b_{\nu'}$ in (5) are effectively modelled by the term $xA_\alpha^\dagger A_\beta$.

In the same spirit as in the previous case, we take as the closest analogue of the ideal boson gas ground state the N q-boson state

$$|N\rangle = \frac{1}{\sqrt{[N]!}}(A_0^\dagger)^N|0\rangle \tag{14}$$

where $[N]! = [N][N-1][N-2]\cdots 1$ is the q-factorial, and

$$[N] = \frac{1-q^{2N}}{1-q^2}. \tag{15}$$

As before, the operator $A_0^\dagger A_0$ is the number operator in the zero deformation limit only. The effect of the deformation can be evaluated taking the expectation value of the $A_0^\dagger A_0$ in the state $|N\rangle$ of equation (14). To evaluate the expectation value, we make use of the result [3]

$$A_\alpha^\dagger A_\alpha = [\hat{N}_\alpha] = \frac{1-q^{2\hat{N}_\alpha}}{1-q^2} \tag{16}$$

where $\hat{N}$ is the number operator in the deformed algebra

$$\hat{N}_0|N\rangle = N|N\rangle. \tag{17}$$

Using the result of (16), one obtains, to lowest order in x,

$$N_0 = \frac{1}{x}\left[1-(1-x)^N\right] \simeq N\left(1 - \frac{1}{2}Nx\right). \tag{18}$$

Comparing this result with the one of equation (10) it is clear that the effect of the deformation is such that

$$Nx \sim Nr_0^3/V \tag{19}$$

that is, the effect of the deformation parameter is proportional to the ratio of the volume occupied by the bosons to the volume of the system. It is clear that when this ratio is small, meaning that there is no considerable overlap of the boson internal wavefunctions, the system behaves as a normal boson gas.

This completes our heuristic discussion on the plausibility of using a q-Heisenberg algebra as a means of treating effectively the internal degrees of freedom of composite particles in a many-body system. Next, we consider the thermodynamics of an ideal q-bose gas [12, 13]. This example is taken to illustrate the effects of the constituent fermions on the thermodynamic properties of a gas of composite bosons. The Hamiltonian of the deformed bose gas is defined [12] as

$$H = \sum_i \epsilon_i A_i^\dagger A_i \tag{20}$$

where $A_i^\dagger$, A_i are, respectively, the creation and annihilation operator of a q-boson in the state of energy ϵ_i. The energy ϵ_i is the kinetic energy plus the internal ground-state energy of the boson.

It follows from equation (16) that the energy eigenvalues of H are given by

$$E(n) = \sum_i \epsilon_i [n_i] = \sum_i E_i(n_i) \tag{21}$$

where $n = \sum_i n_i$ and n_i are the occupation numbers associated with the state of energy ϵ_i. In order to study the thermodynamics of the deformed system we evaluate the grand canonical partition function:

$$Z = \mathrm{Tr}\, \mathrm{e}^{-\beta(H-\mu\hat{N})} = \mathrm{e}^{-\beta\Omega} \tag{22}$$

where $\beta = 1/kT$, μ is the chemical potential and $\hat{N}$ is the number operator. It follows from equations (20) and (22) that in the representation where the Hamiltonian is diagonal:

$$Z = \prod_i Z_1(i, \beta, \mu) \tag{23}$$

with

$$Z_1(i, \beta, \mu) = \sum_{n_i=0}^{\infty} \mathrm{e}^{-\beta(E_i(n_i)-\mu n_i)}.$$

As the exact calculation of Z_1 is not possible, we consider its expansion in terms of the parameter x, where we recall that $q^2 = 1 - x$. (Note that this corresponds to an expansion in the density of the q-gas.) In order to carry out such expansion we note that

$$[n] = \frac{1-q^{2n}}{1-q^2} = \sum_{k=1}^{n} (-1)^{k-1} \binom{n}{k} x^{k-1}.$$

From the equation above and equation (23) we obtain for the expansion of Z_1 up to second order in x the following result:

$$\begin{aligned} Z_1(i, \beta, \mu) = Z_0(z, y_i) \big[1 + y_i (z\mathrm{e}^{-y_i})^2 Z_0^2(z, y_i) x + \left(\tfrac{1}{2} y_i^2 + (3y_i - 1) y_i z\mathrm{e}^{-y_i} Z_0(z, y_i)\right. \\ \left. + 3y_i^2 (z\mathrm{e}^{-y_i})^2 Z_0^2(z, y_i)\right) (z\mathrm{e}^{-y_i})^2 Z_0^2(z, y_i) x^2 + \cdots \big]. \end{aligned} \tag{24}$$

In the above the usual definitions of fugacity $z = \mathrm{e}^{\beta\mu}$ and $y_i = \beta\epsilon_i$ have been used and

$$Z_0(z, y_i) = \sum_{n=0}^{\infty} (z\mathrm{e}^{-y_i})^n = \frac{1}{1 - z\mathrm{e}^{-y_i}}.$$

From equations (22), (23) we obtain for $\beta\Omega$, up to second order in x,

$$\begin{aligned} \beta\Omega = &- \sum_i \log Z_0(z, y_i) - \sum_i y_i (z\mathrm{e}^{-y_i})^2 Z_0^2(z, y_i) x \\ &- \sum_i \left[\frac{y_i^2}{2} (z\mathrm{e}^{-y_i})^2 Z_0^2(z, y_i) + (3y_i - 1) y_i (z\mathrm{e}^{-y_i})^3 Z_0^3(z, y_i) \right. \\ &\left. + \frac{5}{2} y_i^2 (z\mathrm{e}^{-y_i})^4 Z_0^4(z, y_i) \right] x^2 + \mathrm{O}(x^3). \end{aligned} \tag{25}$$

Proceeding as usual, we consider the system contained in a large container of volume V, and replace the summations by an integral:

$$\sum_i f(\epsilon_i) \to \frac{V}{(2\pi)^3} \int \mathrm{d}^3k f(k).$$

We take for the kinetic energy of the boson the non-relativistic expression $\epsilon_i = \epsilon_i(k) = \gamma k^2$, where $\gamma = 1/2m$. In the case of a composite boson one could have, in addition to the kinetic energy, internal excitation energies. Our choice of ϵ_i represents the energy spectrum of composite bosons in their internal ground states. Since the constant internal ground-state energy of the bosons does not play any role in the thermodynamic properties of the system, one needs to consider only the kinetic energy spectrum. Thus the pressure per unit volume can be obtained straightforwardly:

$$\beta p \equiv -\beta\Omega = a\left\{g_{5/2}(z) + \tfrac{3}{2}\left[g_{3/2}(z) - g_{5/2}(z)\right]x + \left[\tfrac{13}{16}g_{1/2}(z) - \tfrac{3}{2}g_{3/2}(z) + \tfrac{11}{16}g_{5/2}(z)\right]x^2 + O(x^3)\right\} \tag{26}$$

where $a = (m/(2\pi\beta))^{3/2}$ and $g_l(z) = \sum_{k=1}^{\infty} z^k/k^l$.

With this, one can obtain the virial expansion of the equation of state. The density, $(n = N/V)$, is obtained by the usual expression:

$$n = \frac{N}{V} = \left(\frac{\partial p}{\partial \mu}\right)_{T,V} = z\left(\frac{\partial \beta p}{\partial z}\right)_{\beta}.$$

Therefore, using equation (26), one obtains

$$n = a\left\{g_{3/2}(z) + \tfrac{3}{2}\left[g_{1/2}(z) - g_{3/2}(z)\right]x + \left[\tfrac{13}{16}g_{-1/2}(z) - \tfrac{3}{2}g_{1/2}(z) + \tfrac{11}{16}g_{3/2}(z)\right]x^2 + \ldots\right\}. \tag{27}$$

In the low-density regime one may write

$$z = a_1\left(\frac{n}{a}\right) + a_2\left(\frac{n}{a}\right)^2. \tag{28}$$

Using this in equation (27), and keeping only terms up to second order in x one obtains:

$$a_1 = 1$$
$$a_2 = -\frac{1}{2^{3/2}}\left(1 + \frac{3}{2}x - \frac{3}{16}x^2\right). \tag{29}$$

Through the substitution of z given in equation (28) into equation (25) the virial expansion is obtained:

$$\beta p = n(1 + Bn + \cdots) \tag{30}$$

where

$$B = -\frac{1}{2^{3/2}a}\left(\frac{1}{2} + \frac{3}{4}x - \frac{21}{32}x^2\right).$$

Note that in the limit of zero deformation, $x = 0$, one obtains the usual result [14]. For finite, small x, one sees that B becomes more negative than in the limit of zero deformation. Thus the deformation has the effect of an attractive potential. This result is easily understood in terms of the interpretation of the deformation parameter as related to the internal fermion degrees of freedom of the composite boson: the Fermi statistics of the constituents cause a depletion of the boson occupation numbers, and in the sum of equation (21) this depletion has the effect of an attractive potential, $\sum_i \epsilon_i[n_i] \leqslant \sum_i \epsilon_i n_i$.

Concluding, we have discussed the possibility of studying many-body problems with composite particles in terms of deformed algebras for the creation and annihilation operators (q-Heisenberg algebras) of the composites. We have considered the example of a gas of bosons and examined the role of the deformation of the algebra of the boson operators. The interpretation of the deformation is that it models the effects of the Pauli principle operating on the constituent fermions. Among other effects, the deformation of the algebra causes the depletion of the single particle occupation of the bosons.

Although we have discussed the example of a system of composite bosons, it is clear that the same methods are applicable to composite fermions. We plan to study such a case in a future publication. Another interesting subject for future work is the study of interacting composite bosons (or fermions). In particular, it would be very interesting to explore the role of the deformation on phase transitions. Such a study might be of interest to superconductivity/superfluidity and quark–gluon plasma phase transitions.

Acknowledgments

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