METHODOLOGICAL NOTES

100 years of the *Uspekhi Fizicheskikh Nauk* journal

Harmony in a many-particle quantum problem

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Abstract. The model quantum problem of a harmonically trapped cloud of identical nonrelativistic particles interacting via a harmonic oscillator potential has an exact solution that can be used to assess the efficiency of approximate methods standardly used in more realistic many-particle calculations.

Keywords: many-particle Schrödinger equation, harmonic oscillator, fermions, bosons, Thomas–Fermi equation

1. Introduction

Physical models are basically a tool to describe and calculate practical situations. In fact, however, real practical situations are generally too complex to allow rigorous calculations, which brings approximate problem-solving methods to the forefront. An efficient way to assess approximations for usefulness and to evaluate the accuracy of the methods is to test them on an exactly solvable model which, even if exotic, allows directly verifying approaches developed for more realistic problems. In other words, exact solutions, which physical problems generally yield only in special degenerate cases, can serve as an excellent test of approximate analysis methods applied to generic cases.

In this paper, we propose a quantum mechanical test model that clarifies and offers visualizations of a large number of approximate methods for systems of many nonrelativistic fermions or bosons, widely exemplified by many-electron atoms (see, e.g., Refs [1–3]) and trapped atomic gas clouds used for the observation of Bose condensation [4, 5]. The advantages of the analytic approaches used (perturbation theory, variational calculus, Thomas–Fermi model, density matrix, collective hydrodynamic description, etc.) are vividly illustrated by a harmonic analogue of such systems, in which interparticle interaction is provided by a linear oscillator potential. This model has a number of remarkable mathematical properties that allow obtaining exact solutions, as if expressly intended for testing standard atomic physics methods, including those for arbitrarily many particles.

The corresponding procedure for obtaining these exact solutions (although apparently not all solutions) is far from new: referred to as 'transformation to normal coordinates', it can be found in nearly any textbook on classical mechanics (see, e.g., Refs [6, 7]), and its quantum extensions are the subject of an extended series of studies by Man'ko and colleagues (Refs [8, 9], to cite just two examples). However, the proposed ideology has not appeared in the available literature, and therefore seems to be of methodological value, as a supplement to an advanced course of quantum mechanics. It should be recognized that despite the many comparisons and parallels drawn below with well-known many-electron systems, this value lies not in furthering the investigation of such systems but only in helping one to master techniques needed in this regard.

2. Problem formulation

We assume that a parabolic potential well representing the field of an atomic nucleus or that of a trap is at rest and contains N identical particles of mass m each, the interaction between them also being parabolic but with a different strength. In one dimension, the steady state of the system is

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described by the Schrödinger equation for the multiparticle wave function

$$-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2\psi}{\partial x_i^2}+\frac{m\omega^2}{2}\left[\sum_{i=1}^{N}x_i^2+\alpha\sum_{i>j}(x_i-x_j)^2\right]\psi=E\psi\,. \tag{1}$$

This, of course, is a pure model situation, with no claim to being real. To repeat, this systems is mainly regarded here as a tool, an instrument intended for instruction purposes rather than an object of investigation (see Section 9, however).

The principal and most remarkable property of the harmonic oscillator is that, as is known, the kinetic and potential energy matrices can always be diagonalized simultaneously in the coordinates $\xi_i(x)$ (which are precisely the ones called 'normal'), with the result that the original Eqn (1) becomes

$$-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2\psi}{\partial\xi_i^2}+\frac{m\omega^2\xi_1^2}{2}\,\psi+(1+N\alpha)\,\frac{m\omega^2}{2}\sum_{i=2}^{N}\xi_i^2\psi=E\psi\,, \tag{2}$$

where we note that because the kinetic energy (or in the quantum domain, the Laplacian) is originally the identity matrix in this case, the new coordinates are orthonormal, i.e., we simply have a rotation, possibly accompanied by some reflections and permutations, of the axes of the multidimensional coordinate system CS-x. The coefficients of the new quadratic form

$$\sum_{i=1}^{N}x_i^2+\alpha\sum_{i>j}(x_i-x_j)^2=\left[1+(N-1)\,\alpha\right]\sum_{i=1}^{N}x_i^2$$

$$-2\alpha\sum_{i>j}x_ix_j\rightarrow\xi_1^2+(1+N\alpha)\sum_{i=2}^{N}\xi_i^2 \tag{3}$$

are easily obtained by an eigenvalue analysis of the $N\times N$ symmetric matrix

$$A=\begin{pmatrix} 1+(N-1)\,\alpha & -\alpha & * & -\alpha\\ -\alpha & 1+(N-1)\,\alpha & * & -\alpha\\ * & * & * & *\\ -\alpha & -\alpha & * & 1+(N-1)\,\alpha \end{pmatrix}$$

because

$$\det\left(A-\lambda E\right)=(1-\lambda)(1+N\alpha-\lambda)^{N-1}$$

(for example, starting from the bottom row and going up, we can subtract from each row its preceding one and then expand the determinant in the unchanged first row). Hence, there are only two eigenvalues: 1 for the vector $\{1,1,\dots,1\}$ (as is easy to verify) and $1+N\alpha$ for all remaining ones.

Therefore, the transition to CS-ξ is easy to perform: once the 'cloud' center-of-mass (CM) coordinates $\xi_1=\left(\sum_{i=1}^{N}x_i\right)/\sqrt{N}$ are segregated (the coefficients here and below are chosen such that the gradient vector normal to a given hyperplane have a unit norm; in fact, a CM coordinate is $1/\sqrt{N}$ times ξ_1 and its square is $1/N$ times ξ_1^2), the remaining axes are constructed in a fully arbitrary way ($(N-1)$-fold degeneracy) by a successive orthonormalization procedure. It is possibly worth choosing some of these axes from among nonoverlapping pairs $(x_i-x_j)/\sqrt{2}$, $i\neq j$, in which case they are automatically orthogonal to one another

and to the first axis, and the corresponding ψ functions are symmetric (antisymmetric) in these pairs at least (see below). For small N, the construction is straightforward: for two particles, we have the exact result

$$\begin{cases}\xi_1=\dfrac{x_1}{\sqrt{2}}+\dfrac{x_2}{\sqrt{2}}\,,\\[2mm]\xi_2=\dfrac{x_1}{\sqrt{2}}-\dfrac{x_2}{\sqrt{2}}\,,\end{cases}\longleftrightarrow\begin{cases}x_1=\dfrac{\xi_1}{\sqrt{2}}+\dfrac{\xi_2}{\sqrt{2}}\,,\\[2mm]x_2=\dfrac{\xi_1}{\sqrt{2}}-\dfrac{\xi_2}{\sqrt{2}}\,,\end{cases}$$

and, for example, for three particles (because it is exactly starting from this case that the axes $\xi_{i\geqslant2}$ allow an arbitrary rotation about the ξ_1 axis and an arbitrary number of permutations; the difference between the left and right CS orientations does not manifest itself in this case).

$$\begin{cases}\xi_1=\dfrac{x_1}{\sqrt{3}}+\dfrac{x_2}{\sqrt{3}}+\dfrac{x_3}{\sqrt{3}}\,,\\[2mm]\xi_2=-\dfrac{\sqrt{2}\,x_1}{\sqrt{3}}+\dfrac{x_2}{\sqrt{6}}+\dfrac{x_3}{\sqrt{6}}\,,\\[2mm]\xi_3=-\dfrac{x_2}{\sqrt{2}}+\dfrac{x_3}{\sqrt{2}}\end{cases}$$

(the inverse transition is also trivial, but we do not discuss it because we do not need it in what follows). Also, for $i=4$, adding the only 'new' axis ξ_4 after the suggested identification of $\xi_1,\xi_2=(x_1-x_2)/\sqrt{2}$, and $\xi_3=(x_3-x_4)/\sqrt{2}$ is straightforward. The coefficients of the matrices relating the old and new coordinates are chosen, as shown above, so as to preserve the Laplacian, and therefore the transition Jacobians everywhere have an absolute value of unity.

Solution (2) for a system of noninteracting oscillators factors in an obvious way:

$$\psi=f(\xi_1)\prod_{i=2}^{N}g_i(\xi_i)\,,\qquad E=\sum_{i=1}^{N}E_i \tag{4}$$

where we use the Hermite polynomials

$$f\propto H_{k_1}\left(\sqrt{\frac{m\omega}{\hbar}}\,\xi_1\right)\exp\left(-\frac{m\omega\xi_1^2}{2\hbar}\right)\,,$$

$$g_i\propto H_{k_i}\left(\sqrt{\frac{m\sqrt{1+N\alpha}\,\omega}{\hbar}}\,\xi_i\right)\exp\left(-\frac{m\sqrt{1+N\alpha}\,\omega\xi_i^2}{2\hbar}\right)\,,$$

$$E=\frac{\hbar\omega}{2}\left[1+2k_1+\sqrt{1+N\alpha}\sum_{i=2}^{N}(1+2k_i)\right]\,,$$

$$k_i=0,1,2,\dots\,. \tag{5}$$

We see that the model parameter α can take arbitrary positive values, but for particles interacting repulsively its magnitude is limited by the inequality $\alpha>-1/N$ (clearly, only for $N\geqslant2$)[1]; otherwise, the external potential cannot hold the cloud of harmonic particles together. It is this solution that we use for comparison with results of approximate methods.

Clearly, the post-factorization diagonalization also applies to the case where particles trapped in an external potential have different α and even different m, but we here discuss only version (1). For nonidentical components, the

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[1] It is instructive (for example, for $N=2$), to trace the appearance of $-1/N$, rather than the apparent $-1/(N-1)$, in the right-hand side of the inequality.

transition to (2) is much more cumbersome and less universal, and is then the end of the story, whereas in the given case it is just the beginning. According to the indistinguishability of quantum objects, a procedure should further be carried out, depending on whether the components obey Bose or Fermi statistics, to symmetrize or antisymmetrize the wave function with respect to all possible permutations $i \leftrightarrow j$ [1, 2, 10], which should be done, first, in the real x-space (not in the formal ξ-space) and, second, for the total wave function, including its spin component, which, due to the spin independence of Hamiltonian (1), arises as a factor in ψ in Eqn (4).

It is well known that for $N \gg 1$, this program, of extreme importance for real atoms and boson traps, can be no less (and in this particular model, even more) challenging to implement than finding ψ. In what follows, we assume for simplicity and in order to be specific that fermions and bosons are spin-1/2 and spin-0 particles, and we let $\uparrow_i (\downarrow_i)$ denote the wave function of the ith fermion with spin up (down). It is also assumed that the fermions interact by repelling ($\alpha < 0$), and the bosons by attracting ($\alpha > 0$) each other. Only problems in one dimension are considered, because another convenient point about the model is the fact that in passing to two or three dimensions, the system is simply diagonalized separately with respect to the x_i and y_i and, if need be, z_i.

3. Mean-field approximation

Available in a variety of versions, the mean-field approximation is apparently the most popular tool for treating $N \gg 1$ many-particle problems, for both statistics of the cloud particles. In atomic physics, it is known as the Thomas–Fermi approximation. We constantly use it in what follows for comparison purposes, and it is worth discussing it in the framework of a model with an interaction potential that does not tend to zero as the interparticle distance tends to infinity.

We stress at the outset that the point is to describe our object (cloud) in a different language by characterizing it by the particle concentration $n(x)$ (thus returning to one dimension) instead of a multiparticle wave function $\psi(x_1, x_2, \ldots, x_N)$. Therefore, for a proper comparison, we must establish a 'dictionary' from one language to the other. Clearly, the indistinguishability of particles allows such a transition to be made by expressing the concentration $n(x)$ as the sum of contributions from each of the particles,

$$n(x) = \sum_{i=1}^{N} \int \cdots \int \left| \psi(x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_N) \right|^2$$

$$\times \, \mathrm{d}x_1 \ldots \mathrm{d}x_{i-1} \, \mathrm{d}x_{i+1} \ldots \mathrm{d}x_N . \tag{6}$$

Because $|\psi|^2$ is symmetric with respect to all x_i, the computations below are quite compact. It is surprising that even very good textbooks either do not present this evident formula at all [1, 2] or give it only in the case of one-electron wave functions [3] (see Section 6), despite clearly losing in terms of connectivity.

Now that we have established the comparison reference for results of the approximate method, it is time to start deriving the formulas of the method. There are two stages to the derivation: the first establishes how the mean or effective field is related to the particle concentration, and the second calculates the 'response' of the cloud to the collective potential profile. The first stage is universal and is independent of whether the potential $\phi(x)$ is produced by a fermion or

boson cloud. It is worthwhile to note here how effective and transparent the harmonic model is as regards writing exact formulas. Because the sum of any number of any quadratic trinomials is a quadratic trinomial, the sought relation is simply

$$\phi = \frac{m\omega^2}{2} \left[x^2 + \alpha \int n(x')(x - x')^2 \, \mathrm{d}x' \right]$$

$$\rightarrow \phi = \frac{m\omega^2}{2} \left[x^2(1 + N\alpha) + N\alpha \langle x^2 \rangle \right] . \tag{7}$$

Here, the concentration distribution moments are assumed to satisfy the relations

$$\int n \, \mathrm{d}x = N, \quad \int x n \, \mathrm{d}x = 0, \quad \int x^2 n \, \mathrm{d}x = N \langle x^2 \rangle ,$$

of which the first is obvious, the third is a tautology, and the second is provable (see below).

On the other hand, bosons and fermions respond differently to the potential because their pressure in the force balance equation

$$-\frac{\nabla P}{n} - \nabla \phi = 0 \tag{8}$$

depends essentially on the statistics. It is commonly assumed that a 'macroscopic' system in its lowest possible energy state has the temperature $T = 0$, and that for a doubly spin degenerate Fermi–Dirac cloud in one dimension, $P = P_{\mathrm{F}} = (\pi\hbar)^2 n^3 / (12m)$, where

$$\frac{3P_{\mathrm{F}}}{2n} + \phi = \mathrm{const} \rightarrow n = \frac{2}{\pi\hbar} \begin{cases} \sqrt{2m(\phi_0 - \phi)}, & \phi < \phi_0 , \\ 0, & \phi > \phi_0 . \end{cases}$$

It follows that n inherits the symmetry of ϕ (the same occurs for the Bose–Einstein statistics), and therefore, if the first moment of n were nonzero, shifting the origin to the point such that $\int n x \, \mathrm{d}x = 0$ would lead to a contradiction due to the presence of an external field in Eqn (7), which loses symmetry as a result of this shift. Finally, using Eqn (7), we obtain

$$n = \frac{2m\omega}{\pi\hbar} \sqrt{1 + N\alpha}$$

$$\times \begin{cases} \sqrt{x_0^2 - x^2}, & |x| < x_0 , \\ 0, & |x| > x_0 \end{cases} \rightarrow \langle x^2 \rangle = \frac{x_0^2}{4} . \tag{9}$$

Thus, the concentration distribution is symmetric with respect to $x = 0$ just because of the external potential that is responsible for the CM of the system. The constants x_0 are determined from the normalization condition

$$\int_{-x_0}^{+x_0} n \, \mathrm{d}x = N = \frac{m\omega}{\hbar} \sqrt{1 + N\alpha} \, x_0^2 .$$

We see that Eqn (9) is simpler and more transparent than the Thomas–Fermi equation for Coulomb-interacting electrons in an atom. In the general case of dimension s,[2] $n \propto (r_0^2 - r^2)^{s/2}$ because $P_{\mathrm{F}} \propto n^{(s+2)/s}$.

Clearly, the main conceptual disadvantage of the averaging approach (which is indeed recognized in the literature) is that the system is described classically, without any signs of

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[2] The dimensionality of concentration depends, of course, on s: n [cm^{-s}].

quantum discreteness [cf. Eqn (5)].[3] Still, some quantum effects can be incorporated quite simply into this approach. For example, to introduce particle tunneling through barriers, an approach widely used currently is to add the gradient of the so-called *Bohm potential*

$$+\frac{\hbar^2}{2m} \nabla \left(\frac{\Delta\sqrt{n}}{\sqrt{n}} \right)$$

to balance equation (8) (albeit for a degenerate plasma rather than bound electrons in an atom [11, 12]). The Bohm potential arises from two factors, the kinetic energy Laplacian in the Schrödinger equation and the $n \leftrightarrow \psi^2$ relation (see Refs [13, 14] for more details). Analytic solution (8) is immediately ruled out in that case, but the corrections introduced are easy to understand. First, because $\phi \propto x^2$ in the system, it follows that in the limit $|x| \to \infty$, the cloud regions with $n \equiv 0$ are replaced by smooth 'wings':

$$-(1 + N\alpha)\left(\frac{m\omega x}{\hbar}\right)^2 \sqrt{n} + \frac{\mathrm{d}^2\sqrt{n}}{\mathrm{d}x^2} \approx 0$$
$$\to n \propto \exp\left(-\frac{m\omega}{\hbar}\sqrt{1 + N\alpha}\, x^2\right),$$

which is by no means surprising, and, second, the Bohm contribution to the 'bulk' of the system is parametrically small:

$$\frac{\hbar^2/(mx_0^2)}{(\hbar n)^2/m} \sim \frac{1}{(nx_0)^2} \sim \frac{1}{N^2}.$$

For Bose–Einstein particles, ignoring temperature effects (excitations) implies that $P = 0$ (see Ref. [15] for more on this). Therefore, a different language is often used here, that employing the Gross–Pitaevskii equation for a certain collective wave function [4, 5], to analyze the situation. Unfortunately, because of the nondecreasing nature of the harmonic interaction potential (for bosons, for which $\alpha > 0$, this potential indeed has the property of confinement), such a language does not appear to apply at all to the model under discussion. On the other hand, it seems totally unnecessary to use deeper and more general descriptions of our purely formal and methodology-oriented model. Still, we can remain in the framework of Eqn (8) by bringing to the fore an effect that appeared above only as a small correction. The harmonic bosons, in striking contrast to fermions, all accumulate on a single level, the lowest one, with all k_i zero, and produce the density profile due exclusively to the Bohm effect:

$$\frac{\hbar^2}{2m\sqrt{n}}\frac{\mathrm{d}^2\sqrt{n}}{\mathrm{d}x^2} - \frac{m\omega^2}{2}\left[(1 + N\alpha)\,x^2 + N\alpha\langle x^2\rangle\right] = \mathrm{const}$$

[cf. Eqn (1)]. If $\mathrm{const} = -\hbar\omega(\sqrt{1 + N\alpha} + N\alpha m\omega\langle x^2\rangle/\hbar)/2$, which is precisely what corresponds to the zeroth, lowest collective level, then

$$n = N\sqrt{\frac{m\omega\sqrt{1 + N\alpha}}{\pi\hbar}}\exp\left(-\frac{m\omega}{\hbar}\sqrt{1 + N\alpha}\, x^2\right)$$
$$\to \langle x^2\rangle = \frac{1}{2\sqrt{1 + N\alpha}}\frac{m\omega}{\hbar}. \qquad (10)$$

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[3] Other approaches exist for incorporating energy discreteness into the description of fermion and boson systems, but their discussion seems out of place here.

It is curious that the potential referred to as the Bohm potential in the fermion community is also known to the boson community, where it is widely used in similar calculations [4, 5], but *is not named in any special way*.

Having dealt with the preliminaries, we now proceed, as planned, to comparing exact and approximate results in various but always harmonic settings.

4. Two harmonic fermions

An object composed of two harmonic fermions is similar to the helium atom, whose relative simplicity has made it a popular testbed for a wide variety of approximate methods [1]. However, whereas real helium allows only a comparison of approximate results with one another, the abstract harmonic system we propose offers an exact result.

Here [see Eqn (5)], the lowest-energy state with $k_1 = k_2 = 0$ can be occupied only by fermions with antiparallel spins (i.e., with an antisymmetric spin function $(\uparrow_1\downarrow_2 - \uparrow_2\downarrow_1)/\sqrt{2}$), for which

$$\psi \propto \exp\left[-\frac{m\omega}{2\hbar}(\xi_1^2 + \sqrt{1 + 2\alpha}\,\xi_2^2)\right]$$
$$= \exp\left\{-\frac{m\omega}{4\hbar}\left[(x_1^2 + x_2^2)(1 + \sqrt{1 + 2\alpha})\right.\right.$$
$$\left.\left. + 2x_1x_2(1 - \sqrt{1 + 2\alpha})\right]\right\}$$

and

$$E = \frac{\hbar\omega(1 + \sqrt{1 + 2\alpha})}{2}.$$

We now compare the last relations with the results of some standard atomic physics approximations.

1. The first-order perturbation theory in α uses the function of a purely external oscillator

$$\psi = \sqrt{\frac{m\omega}{\pi\hbar}}\exp\left[-\frac{m\omega}{2\hbar}(x_1^2 + x_2^2)\right],$$

and yields the energy shift with respect to the basic $\hbar\omega$ contribution,

$$\Delta E = \alpha \iint \psi^2 \frac{m\omega^2(x_1 - x_2)^2}{2}\,\mathrm{d}x_1\,\mathrm{d}x_2 = \frac{\alpha\hbar\omega}{2},$$

i.e., $E = \hbar\omega(1 + \alpha/2)$.

2. In the variational approach, we start by introducing an arbitrary core 'charge' in the form of a factor β in front of ω in the 'unperturbed' ψ function mentioned above (the field of an external oscillator is in a way screened in part by the cloud of particles) and write the expression

$$E = \min_{\beta} \iint \psi^* \hat{H}\psi\,\mathrm{d}x_1\,\mathrm{d}x_2$$
$$= \min_{\beta}\left[\hbar\omega\left(\beta + \frac{1 - \beta^2 + \alpha}{2\beta}\right)\right] = \hbar\omega\sqrt{1 + \alpha},$$

where $\hat{H}$ is the total Hamiltonian in Eqn (1). The method provides the best approximation to the true energy of the system, even though its discrepancy is also of the order $O(\alpha^2)$.

3. The mean-field description, an analog of the Thomas–Fermi picture, turns out to be not that bad after all (even though 2 can hardly be considered a large number):

$$n = \frac{2m\omega}{\pi\hbar} \sqrt{1+2\alpha} \sqrt{x_0^2 - x^2}, \quad x_0^2 = \frac{2\hbar}{m\omega} \frac{1}{\sqrt{1+2\alpha}}$$

[cf. Eqn (9)], which has a remarkable qualitative similarity (compare the width and the value at zero) to the exact result

$$n = \int \psi^2(x, x_2) \, dx_2 + \int \psi^2(x_1, x) \, dx_1$$

$$= 2\sqrt{\frac{2m\omega\sqrt{1+2\alpha}}{\pi\hbar(1+\sqrt{1+2\alpha})}} \exp\left(-\frac{m\omega}{\hbar} \frac{2\sqrt{1+2\alpha}}{1+\sqrt{1+2\alpha}} x^2\right),$$

especially considering the Bohm wings. In addition, the energy of the cloud turns out to be well approximated: adding the kinetic and potential energies of the degenerate one-dimensional harmonic 'gas' gives

$$E = \int \left[\frac{P_F}{2} + n\left(\phi_{ext} + \frac{\phi_{int}}{2}\right)\right] dx = \hbar\omega\sqrt{1+2\alpha}$$

(we have divided effective potential (7) into two parts: an external part and an 'internal' self-consistent part, the one which is proportional to α). The discrepancy is only of the order $O(\alpha)$, however.

The measure of the quantitative nature of the approximation can be assessed by noting that the lowest level, $k_1 = k_2 = 0$, can also be populated by two bosons, for which the mean-field cloud concentration is described by Eqn (10). Again, there is some similarity, but only for moderately large α (although allowing $\alpha > 0$ for fermions, we encounter the same problem). In Section 7, we discuss why the averaging approach is dramatically at odds with the exact solutions for $N\alpha \gg 1$, $\alpha \gg N$.

As another advantage of the harmonic pair, we can clearly observe the exchange-induced level splitting, a possibility that occurs because the symmetrization/antisymmetrization procedure is trivial for a pair. (All the effects can be found in textbooks [1, 2], but in perturbation theory terms). All we need is to take a look at the excited states of the system. For antiparallel-spin fermions (and for bosons), the excited states necessarily include those with even k_2 (for any k_1): the exponentials in Eqn (5) are always symmetric under permutations $x_1 \leftrightarrow x_2$ (as are the Hermite polynomials in f) while being antisymmetric for g for odd k_2. In contrast, in a system with aligned spins (i.e., with the spin function

$$\uparrow_1\uparrow_2 \ \bigvee \ \frac{\uparrow_1\downarrow_2 + \uparrow_2\downarrow_1}{\sqrt{2}} \ \bigvee \ \downarrow_1\downarrow_2$$

to choose from), only odd k_2 are possible. Hence, at the first excited level (compared with the zeroth level, if the spin function is fixed, then this is not an excited but rather the ground level for the system with parallel spins), the energy of the system can take the following values (in units of $\hbar\omega/2$ and at a sufficient distance α from the critical value $-1/2$):

$$1 + 3\sqrt{1+2\alpha} \ (\uparrow\uparrow) \ \bigvee \ 3 + \sqrt{1+2\alpha} \ (\uparrow\downarrow)$$

(we use an obvious short notation for the spin-one and spin-zero states), and the concentration distribution in the fermion cloud

$$n \propto \left(\frac{4\sqrt{1+2\alpha}}{1+\sqrt{1+2\alpha}} \zeta^2 + C\right) \exp\left(-\frac{2\sqrt{1+2\alpha}}{1+\sqrt{1+2\alpha}} \zeta^2\right)$$

(here and hereafter, we set $\zeta = x\sqrt{m\omega/\hbar}$ for brevity) is also found to be different:

$$C = \begin{cases} (1+2\alpha)^{1/2} & (\uparrow\uparrow) \\ (1+2\alpha)^{-1/2} & (\uparrow\downarrow) \end{cases}.$$

However, for $\alpha < -3/8$, the first excited state in the antiparallel case is the level with $k_1 = 0$ and $k_2 = 2$: $E = \hbar\omega(1+5\sqrt{1+2\alpha})/2$, and the difference in n much more pronounced.

5. Three harmonic fermions

As the classics say ([1], see also [10]), passing to $N \geqslant 2$ dramatically complicates the symmetrization of the total wave function. The formulas become increasingly cumbersome, and therefore, here and hereafter, the coefficients in front of ψ and n in exact relations are not given in general, because they can be easily obtained by normalizing to unity or N, respectively.

In the new system, we can no longer set $k_i = 0$ in the lowest state because the resulting wave function is symmetric with respect to the three x_i, a circumstance no spin component can compensate for. Hence, we should allow a shift by unity in one of the quantum numbers, and necessarily in one of $k_{2,3}$ because any f_{k_1} is symmetric anyway (see above) (in the case of repulsion, this is also more favorable). Indeed, we note that if the $\mathbf{k} = \{0, 1, 0\}$ and $\{0, 0, 1\}$ states (where k_i are represented by the components of a certain vector) are made to interfere, a totally antisymmetric function can be constructed. For example, for spins $\uparrow\uparrow\downarrow$, i.e., with the total spin $1/2$, omitting the symmetric exponential factor, this function has the form

$$(x_1 - x_2)\uparrow_1\uparrow_2\downarrow_3 + (x_2 - x_3)\downarrow_1\uparrow_2\uparrow_3 + (x_3 - x_1)\uparrow_1\downarrow_2\uparrow_3 .$$

Therefore, in the ground state of the cloud triple, $E = \hbar\omega(1 + 4\sqrt{1+3\alpha})/2$ and

$$n(x) \propto \iint (x^2 + y^2 + z^2 - xy - xz - yz)$$

$$\times \exp\left\{-\frac{m\omega}{3\hbar}\left[(x^2 + y^2 + z^2)(1 + 2\sqrt{1+3\alpha})\right.\right.$$

$$\left.\left. + 2(xy + xz + yz)(1 - \sqrt{1+3\alpha})\right]\right\} dy \, dz$$

[when ψ is squared, the cross terms disappear due to the orthogonality of the spin functions (cf. Section 6)]; here, y and z are just convenient integration variables, not a real ordinate and a real applicate. It is more efficient to integrate with respect to $\eta_{1,2} = (y \pm z)/\sqrt{2}$, which gives

$$n \propto \left(1 + \sqrt{1+3\alpha} + \frac{6\sqrt{1+3\alpha}}{2+\sqrt{1+3\alpha}} \zeta^2\right)$$

$$\times \exp\left(-\frac{3\sqrt{1+3\alpha}}{2+\sqrt{1+3\alpha}} \zeta^2\right).$$

It is easy to see that unlike the concentration in the preceding example, now, for $\alpha < 0$, n also has a minimum at

zero, which appears natural considering the mutual repulsion of the particles.

Increasing N further leads to even lengthier calculations, and we therefore terminate our discussion of fermions in Section 6.

6. Noninteracting fermions

The case $\alpha = 0$ demonstrates a surprising correspondence between the exact and mean-field descriptions (cf. Section 4). According to the exact description, in the ground state the harmonic particles are in antiparallel-spin ($\uparrow\downarrow$) pairs at each level of the external oscillator (the ψ are expressed in terms of 'one-particle' functions), and therefore the concentration of the cloud is found as the sum of squares of the standard oscillator wave functions, and a compact result is obtained for an arbitrary number of particles. Taking $N = 2K$ for simplicity obviously gives (with all the coefficients preserved [1])

$$n = 2\sqrt{\frac{m\omega}{\pi\hbar}}\exp\left(-\zeta^2\right)\sum_{i=0}^{K-1}\frac{H_i^2(\zeta)}{2^i i!}$$

$$= \sqrt{\frac{m\omega}{\pi\hbar}}2K\frac{\exp(-\zeta^2)}{2^K K!}\left[H_K^2(\zeta) - H_{K-1}(\zeta)H_{K+1}(\zeta)\right]$$

(the interference terms arising in the ψ function that is antisymmetric in the x_i vanish due to the orthogonality of the eigenfunctions, including the spin ones). The above formula for the sum, which can be found in Ref. [16], is easily verified by induction by using the recurrence relation for Hermite polynomials. For example, for $N = 10$,

$$(16\zeta^8 - 64\zeta^6 + 120\zeta^4 + 45)\frac{\exp\left(-\zeta^2\right)}{12\sqrt{\pi}}\sqrt{\frac{m\omega}{\hbar}}.$$

According to the Thomas–Fermi approximation (disregarding the Bohm potential),

$$n = \frac{2}{\pi}\sqrt{N - \zeta^2}\sqrt{\frac{m\omega}{\hbar}}.$$

If K is also zero, i.e., $N = 4M$, the respective exact and mean-field values of the dimensionless concentration $\tilde{n} = n\sqrt{\hbar/(m\omega)}$ at zero can be written as

$$\frac{4M}{2^{2M}\sqrt{\pi}}\frac{(2M)!}{(M!)^2}, \qquad \frac{4\sqrt{M}}{\pi},$$

and are very close because using Stirling's factorial formula $Q! \approx \sqrt{2\pi Q}\exp\left(-Q\right)Q^Q$ shows that they are identical, and this formula is a good approximation even for small Q. For odd K and even for odd N, the two quantities also tend to be identical, although the formulas are somewhat more cumbersome. The system energies calculated from the exact and Thomas–Fermi models are also in agreement: they are given by the respective formulas

$$E = \int\left(\frac{P_F}{2} + n\phi\right)\mathrm{d}x = \frac{N^2\hbar\omega}{4},$$

$$E = \hbar\omega\sum_{i=0}^{K-1}(1 + 2i) = K^2\hbar\omega$$

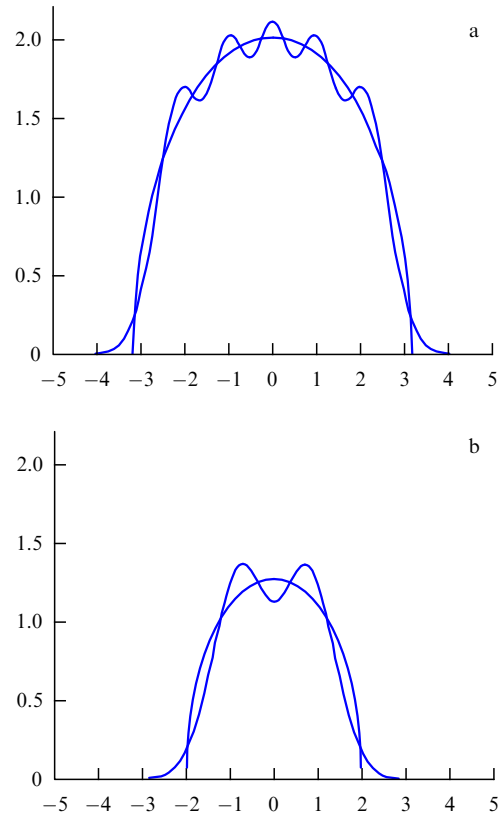(again, for even N for simplicity) (see Section 4).

Figure. Comparison of the predictions of the exact and averaging descriptions for the concentration profile of a cloud of noninteracting fermions for (a) $N = 10$ and (b) $N = 4$.

How close the two descriptions are is illustrated graphically by the profiles $\tilde{n}(\zeta)$ for $N = 10$ and $N = 4$ (see the figure). Of course, the Thomas–Fermi approximation fails to grasp the (very small) oscillations (the so-called shell structure), but it describes the wings of the exact Bohm solution very well. The reason for choosing the smaller variant is that for $\alpha = 0$, it is the quartet, not the triplet, which shows a minimum in the cloud concentration at zero. As N increases, this minimum alternatingly turns into a maximum and reoccurs as a minimum.

7. Harmonic bosons

When harmonic bosons have all dropped to the lowest level $\forall k_i = 0$, i.e., when the system energy is $E = \hbar\omega\left[1 + (N - 1)\sqrt{1 + N\alpha}\right]/2$, the total (fortunately, spinless) wave function is purely Gaussian,

$$\psi \propto \exp\left\{-\frac{m\omega}{2\hbar}\left[\xi_1^2 + \sqrt{1 + N\alpha}\sum_{i=2}^{N}\xi_i^2\right]\right\},$$

where, importantly for the further discussion, $\xi_1 = \sum_{i=1}^{N}x_i/\sqrt{N}$.

To determine $n(x)$, we should first represent the square of this expression as a function of x_i using the equivalence stated in Eqn (3) between the quadratic forms in x and ξ spaces (namely, using it to calculate $\sum_{i=2}^{N}$ in terms of x_i and ξ_1). We should next make the replacement $x_N \to x$ in such ψ^2 using the $x_i \leftrightarrow x_j$ symmetry and then, finally, integrate the resulting exponential with the index

$$- \frac{m\omega}{\hbar N} \left\{ \left[1 + (N-1)\sqrt{1+N\alpha} \right] x^2 \right.$$
$$+ 2(1 - \sqrt{1+N\alpha})\, x \sum_{i=1}^{N-1} x_i$$
$$+ \left[1 + (N-1)\sqrt{1+N\alpha} \right] \sum_{i=1}^{N-1} x_i^2$$
$$\left. + 2(1 - \sqrt{1+N\alpha}) \sum_{i>j} x_i x_j \right\} \tag{11}$$

with respect to the remaining $N-1$ x_i.

The last operation is conveniently carried out in the CS-η, which diagonalizes the form expressed by the underlined terms in Eqn (11). The calculation only requires taking into account that $\eta_1 = \sum_{i=1}^{N-1} x_i / \sqrt{N-1}$, and the eigenvalue of this vector is easily found from the form of the original $(N-1) \times (N-1)$ matrix B of that form:

$$\begin{pmatrix} 1 + (N-1)\sqrt{1+N\alpha} & 1 - \sqrt{1+N\alpha} & * \\ 1 - \sqrt{1+N\alpha} & 1 + (N-1)\sqrt{1+N\alpha} & * \\ * & * & * \end{pmatrix}$$
$$\times \begin{pmatrix} 1 \\ 1 \\ * \end{pmatrix} = (N - 1 + \sqrt{1+N\alpha}) \begin{pmatrix} 1 \\ 1 \\ * \end{pmatrix}.$$

The coefficients of the other η_i^2 are unimportant because the integration over these variables yields only an insignificant pre-exponential factor (see Section 5), but it is clear that similarly to the eigenvalues of the matrix A, they are all equal to $N\sqrt{1+N\alpha}$. Finally,

$$n(x) \propto \exp\left(- \frac{m\omega}{\hbar} \frac{N\sqrt{1+N\alpha}}{N - 1 + \sqrt{1+N\alpha}} x^2 \right). \tag{12}$$

We see that for a cloud of $N \gg 1$ harmonic bosons, the coefficient of ζ^2 in the exponent is the *harmonic* mean of N and $\sqrt{1+N\alpha}$. Is this accidental?

Comparing Eqns (12) and (10) again raises the question that was addressed in Section 4 but postponed until now: Why does the mean-field approximation perfectly correspond to the exact formulas for $N \gg \alpha$ while dramatically failing for $\alpha \gg N \gg 1$? The answer amounts to the following quantitative explanation of the observation of the 'harmonic mean' scaling.

If N is increased for a fixed $\alpha > 0$, at the point where the leading contribution to the confining field comes from the harmonic particles, $N\alpha \gg 1$, the kinetic and potential energies of each particle are comparable, $\hbar^2/(mx_0^2) \sim m\omega^2 N\alpha x_0^2$, according to the virial theorem and based on a simple estimate of terms in Eqn (1) (here, x_0 is the characteristic width of $n(x)$, with $x_0^2 \sim \hbar/(m\omega\sqrt{N\alpha})$). If we fix $N \gg 1$ and infinitely increase α, the cloud structure remains the same as described above until particle collectivization reaches its logical limit by turning the particle ensemble into a 'superparticle' of mass Nm and charge N. From this point on, the observed width n is determined exclusively by the dynamics of this superparticle in the external field, irrespective of the interaction of its internal components,[4] and hence, according to the new virial theorem $\hbar^2/(Nmx_0^2) \sim Nm\omega^2 x_0^2$, we have $x_0^2 \sim \hbar/(m\omega N)$. This regime becomes dominant if the

[4] Analogously, the behavior of an electrostatically trapped proton is unrelated to the dynamics of its component quarks.

Heisenberg 'blurring' of the superparticle exceeds its internal size, i.e., precisely when $\alpha > N$ [the 'blurring' of ξ_1 is ~ 1 according to Eqns (2) and (5)].

The first excited state of a boson system exhibits the same features. For $\alpha > 0$, this state is $\hbar\omega$ ($k_1 = 1$, $k_{i \geqslant 2} = 0$) apart from the ground state, and its wave function, unlike that indicated, has the factor ξ_1, which in $n(x)$ generates the factor

$$\frac{N(1+N\alpha)}{N - 1 + \sqrt{1+N\alpha}} \zeta^2 + \frac{N-1}{2}$$

in front of the already calculated exponential. For $N \gg \alpha \gg 1$, the contribution from the ζ^2 term is small as $\sqrt{\alpha/N}$; however, for $\alpha \gg N \gg 1$, the concentration profile undergoes a strong modification (in terms of the same parameter, which is large in that case) and is determined by the first excited level of the superparticle in the external field. In other words, for $N\alpha \gg 1$, the averaging approach misses the external potential on the background of the collective one and therefore fails to describe the formation of a united harmonic 'fist' at $N \gg \alpha$.

The situation can also be analyzed by using a different parameter variation scheme, namely, by fixing the number of cloud particles and their interaction strength $\alpha\omega^2 = \tilde{\omega}^2 = \text{const}$ and varying the cloud-confining field ω. Then, if we increase the 'rigidity' of the oscillator, i.e., if we try to 'squeeze' the cloud into an increasingly narrow well, the scaling relation $x_0^2 \sim \hbar/(mN\omega)$ suggests that an instant ($N\omega^2 > \tilde{\omega}^2$) is inevitably reached when the width $n(x)$ ceases to decrease and starts to be determined by the internal size of the superparticle, $x_0^2 \sim \hbar/(m\sqrt{N\tilde{\omega}^2})$. After that, the united fist ensemble resists compression successfully for quite a long time, but increasing ω further for $\omega^2 > N\tilde{\omega}^2$ leads to its destruction by the external field and, starting from that moment, the cloud is again compressed according to the $x_0^2 \sim \hbar/m\omega$ law.

The above discussion suggests that the mean-field model is easily corrected 'by hand'. According to Eqn (2), we only need to separate the external oscillator from all the others: first, for $N\alpha \gg 1$, to consider the formation of the collective cloud and then to investigate the motion of its CM in the external potential.

8. Coherent states

One further and still unexploited property of the harmonic oscillator is that the isochronous nature of its dynamics allows the nontrivial evolution of the system to be represented in terms of so-called coherent states [1]; this very simple representation is 'semiclassical' in form and is in fact exact and very efficient. Much of the literature on Bose condensation in magnetically trapped atomic gases [4, 5] has focused on various vibration modes of the clouds of these gases. Most analyses use the hydrodynamics approximation in the collective Gross–Pitaevskii equation; this approximation, as indicated above, is totally inapplicable to the harmonic scenario we advocate here (because of the nonlocal interparticle interaction, such a cloud gas is fully nonideal). The positive side, however, is that this approach allows the exact and sufficiently compact study of the oscillations.

The coherent states of the oscillator are described by the nonstationary wave function

$$\propto \exp\left[\frac{i\bar{p}q}{\hbar} - \frac{m\Omega(q - \bar{q})^2}{2\hbar} - \frac{i\Omega t}{2} - \frac{i\bar{p}\bar{q}}{2\hbar} \right],$$

where Ω is the oscillator frequency and the 'average' coordinate and momentum are functions of time satisfying the classical equations

$$m\dot{\bar{q}} = \bar{p}, \quad \dot{\bar{p}} = -m\Omega^2\bar{q} \;\rightarrow\; \frac{\bar{p}^2}{2m} + \frac{m\Omega^2\bar{q}^2}{2} = \bar{k}\hbar\Omega \,,$$

and hence, if $\bar{q} = \sqrt{2\bar{k}\hbar/(m\Omega)}\,\sin(\Omega t)$, then $\bar{p} = \sqrt{2\bar{k}m\hbar\Omega}\,\cos(\Omega t)$. The quantity $\bar{k}$ is called the 'mean number of quanta.'[5] Unfortunately, using the above exact solution of the Schrödinger equation for a single oscillator in factorizable system (2) of many oscillators involves an unwieldy symmetrization (antisymmetrization) procedure. We therefore use the simplest, two-particle model to demonstrate the method.

If the coherence property is assumed for the first oscillator, $q = \xi_1$, $\Omega = \omega$ (where we use the old notation for the 'means'), and the second, with the coordinate ξ_2, is in the stationary state $k_2 = 0$ (we multiply g by $\exp(-iE_2t/\hbar)$ for completeness) [see Eqn (5)], then the total coordinate function is symmetric and hence describes oscillations of a harmonic cloud of either two bosons or two antiparallel-spin fermions. In this case,

$$n(x,t) \propto \exp\left[-\frac{2\sqrt{1+2\alpha}}{1+\sqrt{1+2\alpha}}\,\frac{m\omega}{\hbar}\left(x - \frac{\bar{q}}{\sqrt{2}}\right)^2 \right].$$

Clearly, this is the antisymmetric oscillation mode involving a CM shift (by $\bar{q}/\sqrt{2}$, as is easy to see), and this result applies straightforwardly to systems with $N > 2$.

If, conversely, $q = \xi_2$, $\Omega = \sqrt{1+2\alpha}\,\omega$, and $k_1 = 0$, then the above version of the system requires that the coherent wave function be preliminarily symmetrized with respect to $x_{1,2}$, giving

$$n(x,t) \propto \left\{ \exp\left[-\frac{2\sqrt{1+2\alpha}}{1+\sqrt{1+2\alpha}}\,\frac{m\omega}{\hbar}\left(x - \frac{\bar{q}}{\sqrt{2}}\right)^2 \right] \right.$$
$$+ \exp\left[-\frac{2\sqrt{1+2\alpha}}{1+\sqrt{1+2\alpha}}\,\frac{m\omega}{\hbar}\left(x + \frac{\bar{q}}{\sqrt{2}}\right)^2 \right] \right\}$$
$$+ 2\cos\left[\frac{2\sqrt{2}\,\bar{p}x}{(1+\sqrt{1+2\alpha})\,\hbar} \right] \exp\left(-\frac{2\sqrt{1+2\alpha}}{1+\sqrt{1+2\alpha}}\,\frac{m\omega}{\hbar}\,x^2 \right.$$
$$\left. -\frac{2\sqrt{1+2\alpha}}{1+\sqrt{1+2\alpha}}\,\bar{k} - \frac{\sqrt{1+2\alpha}\,m\omega}{\hbar}\,\bar{q}^2 \right). \quad (13)$$

This oscillation mode is already symmetric (the expression in curly brackets in the right-hand side) and has a different frequency. As $\bar{k}$ increases, the cosine interference term rapidly decreases to zero.

For a system of parallel-spin fermions, the first mode written above is absent, whereas in the second mode, the antisymetrization of the coherent wave function does nothing more than change the sign of the cosine. We note, however, that scenarios with $k_i \neq 0$ in the stationary part of the total wave function and with coherence with respect to both $\xi_{1,2}$ bring more diversity to life.

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[5] The alternative averaging procedure (i.e., the transition $\bar{*}^2 \rightarrow \overline{*^2}$) does add the correct term $\hbar\Omega/2$ to the energy [1], but this modification of notation is of no importance to us here.

9. Conclusion

The analysis performed shows that the harmonic world is a perfect test ground for approximate methods describing many-particle quantum systems. The approach can play an especially useful role in teaching these methods, because it allows manipulating the necessary calculations in a visual and technically unsophisticated way. At the same time, as a means of acquiring experience in solving potential practical problems, this approach appears to be somewhat inconsistent with the discussion in Section 2 or its implications, and can itself become a subject of physical interest due to its demonstrating very interesting and nontrivial internal physics, as exemplified by the formation of superparticles.

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