Rotating quantum liquids crystallize

To cite this article: S M Reimann et al 2006 New J. Phys. 8 59

View the article online for updates and enhancements.

You may also like
- Entanglement in N-harmonium: bosons and fermions
  C L Benavides-Riveros, I V Toranzo and J S Dehesa
- Generalized Gibbs ensemble in integrable lattice models
  Lev Vidmar and Marcos Rigol
- Andreev-reflection and Aharonov–Bohm dynamics in atomtronic circuits
  Tobias Haug, Rainer Dumke, Leong-Chuan Kwek et al.

Recent citations
- O. E. Alon et al
- Enhanced many-body effects in the excitation spectrum of a weakly interacting rotating Bose-Einstein condensate
  Raphael Beinke et al
- Spontaneous spin polarization in quantum wires
  A.A. Vasilchenko
Rotating quantum liquids crystallize

S M Reimann\textsuperscript{1}, M Koskinen\textsuperscript{2}, Y Yu\textsuperscript{1} and M Manninen\textsuperscript{2}

\textsuperscript{1} Mathematical Physics, Lund Institute of Technology, SE-22100 Lund, Sweden
\textsuperscript{2} NanoScience Center, Department of Physics, FIN-40014 University of Jyväskylä, Finland
E-mail: matti.manninen@phys.jyu.fi

New Journal of Physics 8 (2006) 59
Received 13 February 2006
Published 19 April 2006
Online at \url{http://www.njp.org/}
doi:10.1088/1367-2630/8/4/059

Abstract. Small crystallites form when finite quantal systems are set highly rotating. This crystallization is independent of the statistics of the particles, and occurs for both trapped bosons and fermions. The spin degree of freedom does not change the tendency for localization. In a highly rotating state, the strongly correlated bosonic and fermionic systems approach to that of classical particles.

Contents

1. The model 2
2. Spinless Wigner molecules 3
3. Effect of spin 6
4. Localization of vortices 8
5. Conclusions 9
Acknowledgments 9
References 9

In molecules and solids, the atoms may organize to well-ordered geometrical structures which largely determine their physical and chemical properties. The single atoms localize in the sense that the position of one atom determines the positions of the other atoms. The situation becomes different when atoms are weakly interacting, as in the case of helium, or trapped, cold atom gases.
At sufficiently low temperatures, the atoms—which may be either bosons [1]–[4] or fermions [5, 6]—may form a delocalized quantum liquid where the identity of the individual atoms has disappeared. In the liquid state, the inter-atom correlation weakens fast with distance, i.e., the position of one atom no longer fixes the positions of distant atoms. The electron gas is the classic example, where the transition from a liquid to a localized ground state may occur: already in 1934, it was predicted by Wigner [7] that in the limit of low densities, the electron gas may have a crystalline phase. Though initially discussed for the bulk, the so-called Wigner crystal may also occur in finite fermion systems. A well-known example is quantum dots [8, 9], small electron puddles in a semiconductor heterostructure, where electron localization has been studied extensively in the last decade [10]–[14]. A strong magnetic field is known to enhance localization even in the high-density limit [15]–[22], confirming the prediction of classical ground-state geometries of charged particles in a two-dimensional harmonic confinement [23, 24].

Leaning on the analogy between strong magnetic fields and rotation of a quantum system, many analogies between the physics of the fractional quantum Hall effect in electron systems and Bose–Einstein condensates at high angular momenta have been drawn [20], [25]–[31]. Laughlin [32] showed that there is an analogy between a classical plasma and the fractional quantum Hall liquid, suggesting localization of electrons in a strong magnetic field. Following this analogy, Manninen et al [20] pointed out the similarity of many-body spectra and particle localization between quantum dots in magnetic fields and finite rotating Bose condensates. The existence of these crystalline boson phases beyond the Gross–Pitaevskii mean-field regime was later confirmed by Romanovsky et al [33], pointing at the analogy with the Tonks–Girardeau [34] transition of the Bose gas in one dimension [35].

In this paper we demonstrate that, more generally, repulsively interacting quantum particles—no matter whether they obey bosonic or fermionic statistics—localize when brought to extreme rotation, forming a rotational analogue to the above-mentioned Wigner crystal at low electron densities. The localization is nearly independent of the interparticle interaction and the statistics of the particles, and also occurs if the spin degree of freedom is considered. In the latter case, the many-body states form a very narrow band, clearly separated from high-lying collective excitations. At low angular momenta (and for large particle numbers), the rotational spectrum correspondingly shows localization of quasi-particles which are identified as vortices [36, 37].

1. The model

Let us consider a number \( N \) of interacting particles confined in a two-dimensional harmonic trap. In the spinless case, the particles may be, for example, bosonic atoms with only one hyperfine species, or polarized spin-1/2 fermions, say electrons with each of them in a spin-up state. Including the spin degree of freedom only increases the phase space. The Hamiltonian is

\[
H = \sum_{i}^{N} \left( \frac{p_i^2}{2\mu} + \frac{1}{2} \mu \omega^2 r_i^2 \right) + \sum_{i < j}^{N} v(|\mathbf{r}_i - \mathbf{r}_j|),
\]

where \( N \) is the number of particles with mass \( \mu \), \( \mathbf{r} = (x, y) \) a two-dimensional position vector, \( \omega_0 \) the oscillation frequency of the confining potential, and \( v(r) \) the repulsive interparticle interaction. We will mainly consider long-range Coulomb interactions, \( v(r) = e^2/4\pi\varepsilon_0 r \), but also demonstrate that a short-range Gaussian interaction \( v(r) = v_0 \exp(-r^2/2\sigma^2) \) results in similar
localization of particles when the system is set rotating. (Note that we do not explicitly include magnetic fields, which in absence of the Zeeman effect only induce the rotation.)

In the harmonic oscillator, the single-particle eigenstates are labelled by the number of radial nodes $n$, and by the angular momentum $l$ and its value with respect to the axis of quantization, $m$. For the lowest-energy states at a given angular momentum $L$, the so-called yrast states [38], maximum alignment $L = M$ restricts the space to states with $n = 0$ and $m \geq 0$. This is equivalent to the so-called lowest Landau level approximation frequently made for electron systems in strong magnetic fields.

The non-interacting, single-particle part of the many-body Hamiltonian contributes an excitation energy $(L + 1) \hbar \omega$ to the ground state. In the lowest Landau level, it is thus sufficient to diagonalize only the interaction part of the Hamiltonian, $V_{\text{int}}(r_i, r_j)$. Consequently, the results are independent of the strength of the confinement (apart from the energy scale). One can obtain the lowest-energy states and the energetically low-lying excitations at a given large value of angular momentum $L$ with high numerical accuracy. Naturally, for repulsive interactions, the interaction energy, $\langle V_{\text{int}} \rangle$, is lowered with increasing angular momentum.

2. Spinless Wigner molecules

Figure 1 shows the many-particle spectra calculated for three particles with Coulomb interaction. The results obtained for bosons (open circles) approach those obtained for fermions (crosses) when the angular momentum increases. (The dots mark the energies obtained by quantizing the classical rotations and vibrations, as explained below.) The yrast line of the three-particle system shows pronounced cusps with period of three units of angular momentum. Such cusp states were discussed earlier in the context of quantum dots at high magnetic fields [15]–[20], [22]. In the above example, they originate from the rigid rotation of a triangular, molecule-like structure of...
the three-body system. The symmetry group of the molecule dictates that a purely rotational state can be obtained at only every third angular momentum [16].

The localization of particles can be confirmed by looking at the interparticle correlations. The insets to figure 1 show the pair correlation functions for three fermions at angular momenta \( L = 15, 16 \) and 17. Clearly, at the cusps in the yrast line, the pair correlation function resembles three localized electrons. In the case of centre-of-mass or vibrational excitation, the peaks of the pair correlation function are smeared out due to the internal motion of the particles.

Let us now analyse the low-energy states in terms of the quantized rotational–vibrational spectrum. When the classical Wigner molecule is set rotating, it expands and the eigenfrequencies of vibrations change. In the case of a rigid rotation, the classical energy is obtained by minimizing

\[
E_{\text{cl}}(L) = \frac{1}{2} \mu \omega_0 \sum_i r_i^2 + \sum_i <j \frac{e^2}{4 \pi \epsilon_0 |r_i - r_j|} + \frac{L^2}{2 \mu \sum_i r_i^2}
\]

with respect to the particle coordinates \( r_i \). However, in determining the classical vibrational frequencies the Coriolis force has to be included. We have chosen to solve the classical vibration frequencies using molecular dynamics. The classical system of particles was first set to rigid rotation, then small random changes to the particle velocities were induced, and finally the eigenfrequencies were determined from Fourier transforms of the interparticle distances. It turned out that for particles with repulsive interactions confined in a harmonic well, the correction due to the Coriolis force is essential as opposed to normal rotating molecules where it only gives a small correction [39]. For example, in the case of three classical electrons in a harmonic trap, the vibrational frequencies of a non-rotating Wigner molecule are \( \sqrt{3} \omega_0 \) and twofold degenerate \( \sqrt{3/2} \omega_0 \). However, at high angular momenta, one frequency approaches zero while the other frequencies approach \( 2 \omega_0 \). (Note that irrespective of the angular momentum a centre-of-mass vibration has always the frequency \( \omega_0 \).)

Figure 1 displays the energies of the purely rotational states as red points. These are followed by a state including centre-of-mass rotation (blue points), and a state where the rigid rotation is accompanied by an internal vibration (green points). The minor difference between the fully quantum-mechanical spectrum and the quantized classical spectrum is caused by neglecting the zero-point energy of the low-energy vibrational mode. In fact, also the low-energy excitations can be explained by multiples of centre-of-mass and vibrational excitations of the quasi-classical molecule. Only at high energies or low angular momenta, where the bosonic spectrum begins to deviate from the fermionic one, does this simple picture lose its accuracy.

The spectrum in figure 1 clearly shows that the low-energy states of three interacting particles confined in a two-dimensional harmonic trap approaches that of three localized particles when the angular momentum of the system increases. Remarkably, the low-lying states at high angular momenta appear identical for bosons and fermions.

To study whether the localization occurs also for larger particle numbers we studied the many-particle spectra of fermions and bosons up to seven particles. In all cases, the spectrum directly reveals the localization and its approach to the classical Wigner crystal energy when the angular momentum increases. Figures 2 and 3 show the oscillations of the interaction energy as a function of angular momentum, comparing fermions with bosons. In both cases, we subtracted a smooth second-order polynomial from the spectra to illustrate the characteristic oscillation of the yrast line as a function of angular momentum. In this example with \( N = 7 \), we observe a clear period of six. This is caused by the sixfold symmetry of the classical configuration [23, 24], with one electron at the centre and the remaining six electrons forming a hexagon around
Figure 2. Energy spectrum of seven polarized electrons in a two-dimensional harmonic trap as a function of the angular momentum. A smooth polynomial is subtracted from the potential to emphasize the oscillations caused by particle localization. The inset shows examples of the pair correlation function.

Figure 3. Energy spectrum of seven bosons in a two-dimensional harmonic trap as a function of the angular momentum. A smooth polynomial is subtracted from the potential to emphasize the oscillations caused by particle localization. The inset shows examples of the pair correlation function. The particles interact with the Coulomb interaction.

The pair correlations shown in the inset confirm this classical geometry. They are displayed for a few points where the energy curve has a downward cusp. The somewhat deeper minima at angular momenta $L = 63$ and $L = 105$ correspond to the fractional quantum Hall liquids with fractions (filling factors) $1/3$ and $1/5$. We notice that for small number of electrons the effect of localization on the spectrum is seen clearly already at $L = 3N(N - 1)/2$ corresponding to the
filling factor \( \nu = N(N - 1)/2L = 1/3 \). For an infinite system it is expected that the transition to a Wigner crystal happens at smaller filling factors of about \( \nu = 1/7 \) [40].

Note that even if the oscillation period is the same for bosons and fermions, there is a phase shift of three angular momenta between these two results. This is caused by the different symmetry requirements of the fermion and boson states, in a similar fashion than, for example, the O\(_{16}\) molecule with bosonic nuclei shows only the odd angular momenta in the rotation spectrum [41].

To illustrate that the localization indeed is caused by the increase of angular momentum, we show in figure 4 the evolution of the pair correlation towards the localized state, beginning with small angular momenta. Two sets of results are shown, one for the Coulomb interaction and one for a short-range Gaussian interaction. In both cases, the pair correlation function of the lowest angular momentum shows no localization, but a smooth particle distribution (corresponding to the so-called maximum density droplet [42] as the finite-size analogue to a quantum Hall liquid at integer filling factor). When the angular momentum increases, the system expands (due to the centrifugal force) and the localization gradually increases towards a Wigner molecule, as also shown in figures 2 and 3 above. Note, however, that the localization is weaker in the case of short-range interactions. The result shown in figure 4 is for fermions, but similar localization and expansion of the cluster of particles is obtained in the case of bosons [33]. The magnetic dipole interaction, which can be realized in atomic condensates [43] has a range \( (1/r^3) \) between the short-range Gaussian and a long-range Coulomb interactions. We thus expect similar localization caused by rapid rotation also to occur in the case of repulsive dipolar interaction.

3. Effect of spin

An important question now is whether the spin degree of freedom, neglected so far, may change the tendency of localization of fermions. Notice that the Hamiltonian (1) is spin-independent and the only effect of spin is to increase the phase space.
Figure 5. Energy spectrum (lowest panel) of four electrons with spin as a function of the angular momentum. The different symbols correspond to different total spin of the system. The upper panel shows the total pair correlation function for the two lowest states at $L = 27$. The centre panel shows the $\uparrow \uparrow$, $\uparrow \downarrow$, and total ($\uparrow + \downarrow$) pair correlations for the $L = 28$, $S = 0$ state, indicating the anti-ferromagnetic coupling of the localized electrons.

Figure 5 shows the energy spectrum for four electrons with spin. The different total spin states are shown with different colours. The fully polarized states (blue asterisks connected by a dashed line) show now a period of four, consistent with a classical geometry where the electrons localize at the corners of a square. When all spin states are allowed, the lowest-energy states form a narrow band, clearly separated from the higher excitations. We argue that these states are a consequence of rigid rotations of the Wigner molecule: now, as spin is included, pure rotations are allowed for any angular momentum due to the spin excitations, which cost nearly zero energy.

The situation is related to that in narrow quantum rings [44, 45]. In strictly one-dimensional rings, the spin and charge degrees of freedom completely separate and the Heisenberg model, together with the quantized rotational–vibrational states, can explain in quantitative detail the whole many-particle spectrum [44]. In the case of a quantum dot, the situation seems to be slightly more complicated: while the Heisenberg model (and group theoretical analysis) still gives the correct spin states for each angular momentum, it does not explain quantitatively the energy differences, i.e. the spin and charge excitations seem not to be completely decoupled.
Figure 6. Pair correlation function of 36 electrons in a harmonic trap with angular momentum $L = 708$ showing the exchange-correlation hole and four vortices (left) and the vortex–vortex correlation function showing that the vortices are well localized (right).

Figure 5 also shows examples of correlation functions. The upper panel shows the total correlation functions for $L = 27$ for the lowest state $S = 1$ and the first excited state $S = 2$. Clearly the state $S = 1$, belonging to the lowest band, shows localization of the electrons. In the excited state, however, the peaks are smeared out due to a centre-of-mass excitation. The middle panel shows the correlation function for the lowest-energy state with $L = 28$. In this case, the total spin is $S = 0$ and the state clearly shows anti-ferromagnetic order and electron localization.

When the number of electrons increases, computations including spin become more demanding, and it is not possible to reach as high angular momenta as in the spectra of figures 2 and 3. However, traces of localization can be seen already at relatively low angular momenta, as indicated in figure 4. We have made further calculations with up to seven particles. In all cases, the results showed a clear separation of the energy band, pointing at electron localization with possible spin-excitations, similar to the four-electron case shown in figure 5.

4. Localization of vortices

Finally, we note that localization by rotation can also happen in the case of quasi-particles, even when they are collective excitations. An example here are the vortex patterns emerging in rotating clouds of bosons or fermions at smaller angular momenta [36, 37, 46]. For clear vortex states, naturally, the number of particles should be much larger than that of the vortex quasi-particles. We are thus limited to study polarized fermions (or spinless bosons). Figure 6 shows the electron–electron pair-correlation function computed for 36 electrons with angular momentum $L = 708$. It should be emphasized that the angular momentum $L = 708$, although a large number, is relatively small. In fact, it corresponds to $L = 24$ for seven particles, where according to figure 4 no localization of particles is expected.

In addition to the exchange-correlation hole around the reference electron, we see four minima in the otherwise smooth density distribution.

The formation and localization of vortices can be understood with help of the electron–hole dualism [37], which also makes it possible to plot the vortex–vortex correlation function (also shown in figure 4). Similar vortex localization was also found in bosonic systems [36], [47]–[49].
5. Conclusions

We have shown that quantum mechanical particles, when set rotating in a two-dimensional harmonic trap, tend to localize to Wigner molecules. The localization is seen clearly in the periodic oscillations in energy spectrum as a function of the angular momentum. The many-particle spectrum can be explained in detail by rigid rotation and vibrational modes calculated using classical mechanics. These results seem universal. They are independent of the shape or range of the interparticle interaction, and fermions and bosons show similar localization. Considering also the spin degree of freedom does not change the tendency for localization. With spin, the many-body states form a very narrow band, clearly separated from high-lying collective excitations. When the particle number is sufficiently large, the rotational spectrum shows localization of quasi-particles which can be identified as vortices.

Acknowledgments

We would like to thank B Mottelson, J Jain and S Viefers for several valuable discussions. This work was supported by the Academy of Finland, the Swedish Foundation for Strategic Research, Swedish Research Council, and the European Community project ULTRA-1D (NMP4-CT-2003-505457).

References

[1] Anderson M H, Ensher J R, Matthews M R, Wieman C E and Cornell E A 1995 *Science* **269** 198
[2] Andrews M R, Mewes M-O, van Druten N J, Durfee D S, Kurn D M and Ketterle W 1996 *Science* **273** 84
[3] Cornall E A and Wieman C E 2002 *Rev. Mod. Phys.* **74** 875
[4] Ketterle W 2002 *Rev. Mod. Phys.* **74** 1131
[5] Greiner M, Regal C A and Jin D S 2003 *Nature* **426** 537
[6] Jochim S, Bartenstein M, Altmeyer A, Hendl G, Riedl S, Chin C, Hecker Denschlag J and Grimm R 2003 *Science* **302** 2101
[7] Wigner E P 1934 *Phys. Rev.* **46** 1002
[8] Chakraborty T 1999 *Quantum Dots: A Survey of the Properties of Artificial Atoms* (Amsterdam: North-Holland)
[9] Reimann S M and Manninen M 2002 *Rev. Mod. Phys.* **74** 1283
[10] Jauregui K, Hausler W and Kramer B 1993 *Europhys. Lett.* **24** 581
[11] Egger R, Hauser W, Mak C H and Grabert H 1999 *Phys. Rev. Lett.* **82** 3320
[12] Yannouleas C and Landman U 1999 *Phys. Rev. Lett.* **82** 5325
[13] Reimann S M, Koskinen M and Manninen M 2000 *Phys. Rev.* **B** 62 8108
[14] Reusch B, Hauser W and Grabert H 2001 *Phys. Rev.* **B** 63 113313
[15] Maksym P A and Chakraborty T 1990 *Phys. Rev. Lett.* **65** 108
[16] Ruan W Y, Liu Y Y, Bao C G, Zhang Z Q 1995 *Phys. Rev.* **B** 51 7942
[17] Maksym P A, Imamura H, Mallon G P and Aoki H 2000 *J. Phys.: Condens. Matter* **12** R299
[18] Maksym P A 1996 *Phys. Rev.* **B** 53 10871
[19] Wójcik A and Hawrylak P 1997 *Phys. Rev.* **B** 56 13227
[20] Manninen M, Viefers S, Koskinen M and Reimann S M 2001 *Phys. Rev.* **B** 64 245322
[21] Jean G S, Chang C C and Jain J K 2004 *Phys. Rev.* **B** 69 241304
[22] Yannouleas C and Landman U 2004 *Phys. Rev.* **B** 70 235319
[23] Bolton F and Rößler U 1993 *Superlatt. Microstruct.* **13** 139
[24] Bedanov V M and Peeters F M 1994 *Phys. Rev.* **B** 49 2667

*New Journal of Physics* **8** (2006) 59 (http://www.njp.org/)
[25] Wilkin N K, Gunn J M F and Smith R A 1998 Phys. Rev. Lett. 80 2265
[26] Wilkin N K and Gunn J M F 2000 Phys. Rev. Lett. 84 6
[27] Viefers S, Hansson T H and Reimann S M 2000 Phys. Rev. A 62 053604
[28] Cooper N R, Wilkin N K and Gunn J M F 2001 Phys. Rev. Lett. 87 120405
[29] Regnault N and Jolicoeur Th 2003 Phys. Rev. Lett. 91 030402
[30] Regnault N and Jolicoeur Th 2004 Phys. Rev. B 69 235309
[31] Chang C C, Regnault N, Jolicoeur T and Jain J K 2005 Phys. Rev. A 72 013611
[32] Laughlin R B 1983 Phys. Rev. B 27 3383
[33] Romanovsky I, Yannouleas C and Landman U 2004 Phys. Rev. Lett. 93 230405
[34] Tonks L 1936 Phys. Rev. 50 955
Girardeau M 1960 J. Math. Phys. 1 516
[35] Kinoshita T et al 2004 Science 305 1125
Paredes B et al 2004 Nature (London) 429 277
[36] Toreblad M, Borgh M, Koskinen M, Manninen M and Reimann S M 2004 Phys. Rev. Lett. 93 090407
[37] Manninen M, Reimann S M, Koskinen M, Yu Yand and Toreblad M 2005 Phys. Rev. Lett. 94 106405
[38] Mottelson B 1999 Phys. Rev. Lett. 83 2695
[39] Landau L D and Lifshitz E M 1958 Quantum Mechanics (London: Pergamon)
[40] Lam P K and Girvin S M 1983 Phys. Rev. B 30 473
[41] Tinkham M 1964 Group Theory and Quantum Mechanics (New York: McGraw-Hill)
[42] MacDonald A H, Eric Yang S-R and Johnson M D 1993 Aust. J. Phys. 46 345
[43] Santos L, Shlyapnikov G V, Zoller P and Lewenstein M 2000 Phys. Rev. Lett. 85 1791
[44] Koskinen M, Manninen M, Mottelson B and S M Reimann 2001 Phys. Rev. B 63 205323
[45] Viefers S, Koskinen P, Singha Deo P and Manninen M 2004 Physica E 21 1
[46] Saarikoski H, Harju A, Puska M J and Nieminen R M 2004 Phys. Rev. Lett. 93 116802
[47] Abo-Shaer J R, Raman C, Vogels J M and Ketterle W 2001 Science 292 476
[48] Butts D A and Rokhsar D S 1999 Nature 397 327
[49] Kavoulakis G M, Reimann S M and Mottelson B 2002 Phys. Rev. Lett. 89 079403