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QUANTUM MECHANICS AT WORK

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Abstract

The paper of N. Bogoliubov [J. Phys. USSR **11**, 23 (1947)] has opened the way to understanding coherent quantum many-body systems. I briefly review current efforts aimed at controlling the quantum world and developing novel applications of the fundamental laws of quantum mechanics, which are todays descendants of his work. I illustrate these efforts with theoretical results obtained at SNS over the last few years.

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1 Background

It is an honour and a pleasure to contribute to this special issue of *Concepts of Physics* dedicated to Professor Bogoliubov on the sixtieth anniversary of his seminal paper on the superfluid gas of neutral Bose particles. His work has been a crucial step in the development of basic understanding of coherence in condensed many-particle systems, and it is especially appropriate to recall it at this time when a widespread research drive is going on in many laboratories with the aim of applying the fundamental laws of quantum mechanics to new progress in basic knowledge, technology, and society.

The basic issues in the study of quantum many-body systems that are of foremost interest in this context fall in the realm of Statistical Physics: mainly Bose-Einstein condensation and the mechanisms for superfluidity in ultracold atomic gases, quantum field theory and quantum phase transitions, models for strongly correlated condensed-matter systems and for cosmic objects, transport phenomena and irreversible processes in quantum fluids and in electron fluids moving through Josephson-junction arrays, random paths and percolation phenomena. Two main areas are at the focus of attention:

1.1 Matter waves, atom optics, and superfluidity [1]

Bose-Einstein condensation was predicted in 1924-25 to occur in a gas when the de Broglie wavelength associated with the average particle momentum becomes comparable with the mean interparticle distance, so that the gas diffracts on itself and starts condensing into a macroscopically coherent state. This work gave birth to quantum statistical mechanics and to the concept of bosons and fermions. The main conceptual achievement of Bogoliubov's work in this area seems to me to be the idea that single-particle excitations at long wavelengths in a Bose-Einstein-condensed gas at zero temperature coincide with collective sound-wave excitations. The rationale behind this fact is that the condensate forms a coherent whole so that ejection or injection of a particle must necessarily be accompanied by the generation of propagating density waves.

Condensation was achieved in the laboratory in 1995 with ultracold gases of bosonic alkali atoms (at temperatures below 10^{-7} K and densities of order $10^{12} - 10^{14}$ atoms/cc), this achievement being awarded the Nobel Prize in Physics in 2002. Condensation has since been achieved in gases of several other atomic species and in a number of trapping configurations, including lattices generated by means of advanced optical techniques. Attention soon turned to ultra-cold fermion gases, with superfluidity *via* condensation of paired fermionic atoms being achieved in 2004. Work on ultracold Fermi gases currently is a most advanced field of endeavour in this area, with the search for novel mechanisms of superfluidity being a main focus of attention. Some such novel mechanisms are expected to be relevant to nuclear physics and to cosmology. An impressive number of experimental and theoretical groups are working worldwide on quantum atomic and molecular gases: a proposal to ESF a few years back showed that some 80 research groups comprising some 300 researchers were active in this area in Western Europe alone. The current low-temperature record is at 500 pK.

1.2 Electrons in nanostructures [2, 3]

Understanding the ground-state properties and the elementary excitations and transport mechanisms of a fluid of interacting electrons has been the basic problem of condensed matter physics ever since the Thomas-Fermi and Wigner-Seitz theories were proposed in the early days of quantum mechanics. The main achievements of the 1950s were the mapping of the Fermi surface for conduction electrons in metals and the Bardeen-Cooper-Schrieffer (BCS) theory, using the Bogoliubov transformation to treat the transition to the superconducting state *via* condensation of weakly bound electron pairs. The 1960's saw the theory of short-range order in the electron gas and the related development of density-functional theory. Further progress in the understanding of the superconducting state was based on the Bogoliubov-de Gennes equations and the Landau-Ginzburg equations.

Main attention since the 1980s has been on electron fluids in reduced dimensionalities inside man-made nanostructures: electrons in quantum wells, quantum wires, carbon nanotubes, quantum dots, and superconductivity in arrays of Josephson junctions. The discovery of the quantum Hall effects in quasi-two-dimensional (2D) electron fluids has brought to light a novel state of matter, on which much work is still being done. Bosonization and the Bogoliubov transformation have been at the root of understanding strongly correlated electron fluids in low dimensionality: here again, as a consequence of 1D topology, the elementary excitations in the low energy sector are the collective oscillations of charge and spin densities. Tests of these theories and their further extensions to novel mechanisms for superfluidity are being developed in atomic quantum gases, where ultra-low temperature, ultra-high purity, and easy tuning of the interactions and of particle concentrations and chemical potentials allow unprecedented control in experimental studies.

I illustrate below the spirit of theoretical research in the areas of electron and atom gases by summarizing some of the research that has recently been carried out on these systems within my group in Pisa. Citations of the ample literature and of other peoples work can be found in each of the references that I give below to our own work. Before starting this presentation, however, I should mention two most important areas of development for theoretically minded young researchers:

1.3 Structure and functional properties of liquids, glasses, and biomolecules by the Car-Parrinello method in molecular dynamics [4]

These studies have been a most important outcome of progress in electron-gas theory. They treat the system microscopically as made of valence electrons and ionic cores, and (in spite of the vastly different time scales for the dynamics of these two components) drive them simultaneously towards global equilibrium by generating atom-core trajectories on the potential-energy hypersurface determined by the self-adjusting electron density. This most powerful statistical-mechanical technique has spread world-wide to innumerable research groups in physics, chemistry, and biology.

1.4 Quantum computing and communication [5]

With the continuing miniaturization of electronic devices, we are approaching the microscopic level where quantum laws dominate. It is expected that by the year 2020 computations will be carried out at the atomic level, where a single electron or a single atom will be used to store one (or more) bits. Novel developments in this area include the entanglement of quantum variables, teleportation of information, cryptography, and the use of the spin variable in quantum transport. These aims have motivated the currently intense study of confined quantum fluids as mentioned under 1.1 and 1.2 above. The search for large-scale, error-free quantum computers is reaching a junction at which condensed-matter physics, knot theory, string theory, anyons, and quantum Hall effects are all coming together.

2 Matter waves and superfluidity

2.1 Single-particle and collective excitations in condensed Bose gases at finite temperature [6]

As recalled above, Bogoliubov proved that the elementary long-wavelength excitations of a condensed Bose gas at zero temperature simultaneously are single-particle excitations and collective density fluctuations: that is, the poles of the single-particle Greens functions and of the density response function coincide in this limit. Later related work treating condensed boson fluids with arbitrarily strong interactions, due to Hugenholtz and Pines and to Gavoret and Nozières, led to exact definitions of the chemical potential and of the superfluid fraction in terms of the single-particle Greens functions, and demonstrated that at zero temperature the single-particle excitation spectrum and the density excitation spectrum are gapless and coincide at long wavelengths. What happens to these functions as the temperature of the Bose-Einstein-condensed fluid is raised towards the critical temperature for condensation?

We have given an answer to this question for the charged-boson gas within the dielectric formalism used by Gavoret and Nozières. The Bogoliubov theory shows that in the boson plasma at zero temperature, as a consequence of the Hugenholtz-Pines relation for the chemical potential, the single-particle pole lies at the collective plasma frequency and is therefore well separated from low-frequency excitations. We carry out explicit calculations in the random-phase approximation (RPA), which is especially suited for a weakly coupled gas with long-range forces. We find that with increasing temperature the single-particle spectrum forms a continuum extending from the transverse mode frequency to the plasma frequency and takes a double-peak structure, whereas the density fluctuation spectrum still contains only a progressively broadening single peak at the plasma frequency. This result can be understood by noticing that, as a growing cloud of thermal excitations comes to accompany the condensate, a new channel of damping through excitation of transverse currents opens up for the single-particle motions, whereas only damping into excitation of longitudinal currents remains active for the density fluctuations. Of course, the coupling between single-particle excitations and density fluctuations steadily decreases with increasing temperature and completely vanishes in the transition to the normal state.

2.2 The BCS-BEC crossover [7]

A key tool in research on ultracold atomic gases is the use of Fano-Feshbach resonances in atom-atom scattering to vary the magnitude and even the sign of the coupling strength by merely tuning an applied magnetic field. In a fermion gas this tool has allowed the exploration of the full range of superfluidity mechanisms running from the BCS regime of weakly bound Cooper pairs to the BEC regime where Bose-Einstein condensation of preformed, tightly-bound molecular dimers is occurring. The intermediate, strongly correlated "unitarity" regime around the resonance, where the coupling changes from attractive to repulsive, currently is the main focus of attention. We have been able to give a microscopic theory of the collective low-frequency excitations of a fermion superfluid inside an elongated harmonic trap across a Fano-Feshbach resonance driving a BCS-BEC crossover, and to compare these theoretical results with the experimental data on the axial and transverse breathing modes of the superfluid that were at the same time being measured in two different laboratories.

The Goldstone theorem predicts that a gapless mode in the long-wavelength spectrum of a superfluid Fermi gas is associated with the broken gauge symmetry. In the BCS limit this is the Anderson-Bogoliubov phonon propagating at the speed of first sound, which evolves into the Bogoliubov sound mode in the BEC limit. In the crossover there is a strong hybridization between these phonon modes. We have used the hydrodynamic equations of an inviscid fluid to evaluate sound-wave propagation in a fermion superfluid inside an elongated harmonic trap from its equation of state, and have proposed an experiment to measure the speed of sound in such a superfluid along the crossover from BCS to unitarity. In the normal state one would instead predict that the gas collapses as the strength of the attractive coupling increases away from the ideal-gas limit.

2.3 Terrestrial black holes [8]

Interest in pursuing terrestrial analogues of gravitational physics in condensed-matter systems has been motivated by a seminal observation by Unruh regarding the analogy between sound-wave propagation in a rotating fluid and propagation of a Klein-Gordon field in a curved space-time. Much like superfluid hydrodynamics is a large-scale effective theory of microscopic superfluids, field theory in a curved space-time might be regarded as a large-scale limit of a possible microscopic formulation of quantum gravity. The crucial point is that, whereas microscopic theories of quantum gravity are still largely a matter of speculation, the microscopic theory of superfluids is well developed, and in particular one may hope that assessing the mechanisms of sound radiation from "terrestrial black holes" beyond the hydrodynamic picture may offer new insights into the microscopic origin of cosmic black-hole radiance, the Hawking effect, and other phenomena predicted in cosmology.

A key step in such an "analogue gravity" program is the study of scattering and radiance phenomena from black holes whose background space-time can be associated with fluid excitations such as vortices. In this viewpoint we have focused on the analogy between black holes and vortices in the so-called "draining-tub geometry": both flow fields are endowed with an event horizon and an ergosphere, the former being a surface which allows only one-way propagation of physical signals and the latter being a shell between the horizon and the surface where the rotational velocity is the speed of signal propagation (light or sound waves, as the case may be). Particles falling into the ergosphere are forced to rotate faster and thereby gain energy, and may still escape because they are outside the event horizon. Thus the rotating fluid can emit energetic particles at the expense of its own energy and part of its energy can be extracted *via* the mechanism of superradiance.

We have studied the superradiant scattering of a quasi – monochromatic sound wavepacket impinging on a hydrodynamic vortex, using novel mathematical tools involving finite-elements methods, excision techniques, and constrained evolution schemes for strongly hyperbolic systems. We have evaluated the dependence of the superradiant energy gain by a wavepacket carrying angular momentum on the angular speed of the vortex and found a very rapid increase of the energy gain at angular speeds that are typical of rotating Bose-Einstein condensates in the laboratory. The "critical" angular speed marks the transition to the regime where the radius of the ergosphere is no longer related to the radius of the event horizon, but starts growing linearly so as to create a growing ergospheric shell where rotational energy can be extracted from.

2.4 Phase equilibria in confined quasi-one-dimensional Fermi gases [9]

As already remarked in Section 1, ultracold atomic gases allow ultraclean and controlled observations testing ideas and methods that were originally proposed for electron fluids in the context of solid-state physics, many-body physics, and astrophysics. Of particular interest are the strongly correlated two-component liquids of fermions in quasi-1D configurations, known as the Luttinger liquid in the case of repulsive interactions and the Luther-Emery liquid in the case of attractive interactions. The properties of 1D fermion fluids are fundamentally different from those of normal Fermi liquids in higher dimensionalities: their elementary excitations are not Landau quasiparticles, but rather collective oscillations of the charge and spin densities, that can propagate at different speeds giving rise to spin-charge separation. According to an argument given by Haldane, the symmetry of a wave function in the 1D fluid (in contrast to higher dimensionalities) cannot be tested by a continuous change of coordinates that exchanges particles without a close approach leading to a collision: thus the effects of the interactions and those of the statistics cannot be separated. Haldane emphasizes that the low-energy properties of the 1D fluid are fixed once its particle density, kinetic mass density, and compressibility are given, and the only remaining difference between Fermi and Bose systems is attributable to the different selection rules on the current quantum numbers. Luttinger-liquid behavior is experimentally established in the physics of electronic transport in quantum-Hall edge states and of quantum spin chains, whereas no observation of the Luther-Emery phase has so far been reported in solid-state electronic systems.

Exact solutions for the ground state of 1D two-component Fermi liquids are available in the absence of axial confinement, based on bosonization and the Bogoliubov transformation. We have lately focused on exposing the structural characteristics of strongly correlated Luttinger and Luther-Emery fluids under axial confinement, with a view to providing predictions that could be tested experimentally in atomic Fermi gases inside elongated traps. We describe the gas by a Hubbard Hamiltonian under cigar-shaped harmonic confinement superposed onto an optical lattice, and evaluate its ground-state density as a function of the coupling strength across a confinement-modified Fano-Feshbach resonance. With repulsive interactions and on varying the filling of the lattice, we have brought to light a series of quantum phase transitions involving equilibria between Luttinger-liquid, Mott-insulator, and band-insulator states, these results being quantitatively confirmed by our Quantum Monte Carlo simulation data. The introduction of disorder, besides smoothing out these phase transitions, makes the gas incompressible at low filling, from suppression of percolation. For attractive interactions we demonstrate formation of a Luther-Emery liquid exhibiting compound phases characterized by the coexistence of spin pairing and atomic density waves. In essence, the confinement pins the phase of density oscillations and exposes their structure as due to the formation of spin pairs associated with the opening of a gap in the spin-density excitation spectrum. We have proposed a diffraction experiment that would reveal the existence of such atomic density waves.

The above presentation refers to symmetric mixtures of two states of fermions (*i.e.* mixtures containing equal numbers of spin-up and spin-down Fermi particles) as in a BCS superconductor, where pairing can be complete and the entire gas becomes superfluid. A further type of tunability is easily available in atomic gases, in which one creates in a controlled way a population imbalance between the two spin species and produces a mismatch between their Fermi surfaces. Beyond a critical spin polarization the gas is observed to consist of a superfluid core surrounded by a cloud of unpaired fermions. There has been in parallel a flurry of theoretical activity on non-conventional superfluid states obtained from pairing in conditions where the Fermi surfaces do not match: this area also has relevant implications for condensed-matter physics (*e.g.* pairing between electron populations in different energy bands), nuclear physics (*e.g.* neutron-proton pairing), and quantum chromodynamics (*e.g.* in relation to mass differences between the strange, up, and down quarks). In this context Liu and Wilczek have proposed the possibility of an "interior-gap" superconducting state, in which the pairing interaction carves out a gap within the interior of a large Fermi sphere while the exterior surface remains gapless. Another example is the Larkin-Ovchinnikov and Fulde-Ferrel (LOFF) inhomogeneous-superfluidity phase, in which the momenta of the pairing fermions do not add up to zero as in the BCS Cooper pair. An immediate consequence is that the superfluid order parameter and the superfluid density vary in space. The original proposal concerned superconductivity in a non-magnetic metal containing magnetic impurities: a first-order transition was proposed to a "breached-pair state", in which partial depairing is produced in momentum space by the spin-exchange field in conjunction with a shift of the Fermi spheres for the two spin populations. This proposal has not yet been confirmed beyond reasonable doubt in condensed matter: its observation would necessitate the use of high magnetic fields and type-II superconductors that should be essentially devoid of impurities.

2.5 Frustration in cold-atom analogues of Josephson-junction arrays [10]

Frustration can be introduced into Josephson junctions arrays (JJA) by applying a magnetic field to modify the energetically preferred phase relationship between neighboring sites: it becomes impossible to attain the optimal phase difference for each bond. Fully frustrated JJAs exhibit a compound phase transition in which an Ising transition associated with discrete broken translational symmetry and a Kosterlitz-Thouless transition associated with quasi-long-range phase coherence occur nearly simultaneously. We have proposed a realization of this system using ultracold atoms on a square optical lattice with modulated frustrating bonds and shown that momentum-distribution measurements could be used to study this incompletely understood phase transition. Phase coherence of cold atoms in an optical lattice can be directly detected by observing a multiple matter-wave interference pattern after ballistic expansion: phase coherence produces a lattice of diffraction peaks, and the combination of coherence and Ising broken translational symmetry leads to additional peaks.

3 Electrons in reduced dimensionalities

3.1 Quasiparticle self-energy in two-dimensional electron liquids [11]

The 2D electron liquid serves as a model for the electronic carriers inside a semiconductor inversion layer or in a quantum well inside a man-made nanostructure. The renormalization of the electron mass by many-body effects and the effective spin susceptibility are important parameters to describe the physical behaviors of an electron fluid inside a quantum well, and have recently been subjected to extensive experimental study. With this motivation we have revisited the microscopic calculation of the quasiparticle self-energy in a 2D electron liquid over a broad range of electron coupling strength, with special attention to the merits of the on-shell approximation, commonly used in weak-coupling situations, versus the self-consistent solution of the Dyson equation in the complex-frequency plane.

In our work we have reconsidered a physically transparent "renormalized Hamiltonian approach" originally proposed by Yarlagadda and Giuliani, in which a few "test electrons" are selected from the electron gas while the remainder is treated as a dielectric screening medium. As the test electrons move through this medium, they produce fluctuations in the charge and spin densities, which in turn dress the test electrons with virtual clothing and screen their mutual interactions. After averaging over the coordinates of the screening medium, an effective renormalized Hamiltonian containing only the degrees of freedom of the clothed test electrons is derived. In essence, the test electrons are viewed in this approach as Landaus Fermi-liquid quasiparticles interacting *via* Kukkonen-Overhauser forces. Our calculations yield two main results: (i) a full solution of the Dyson equation soon proves necessary to obtain a well-defined effective mass as the Coulomb coupling strength is increased in the 2D fluid; and (ii) inclusion of both charge- and spin-density short-range order is crucial to obtain reasonable agreement with the measurements.

3.2 Electron structure of quantum dots [12]

A common way to fabricate a quantum dot in the laboratory is to restrict the 2D electron gas inside a semiconductor heterostructure by creating a bowl-like potential in which some number of electronic carriers are trapped. The number of electrons and the properties of the dot can be varied in a controlled way by means of electrostatic gates, changes in geometry, or applied magnetic fields. The confinement introduces a new length scale and the quantum dot can be viewed as an artificial atom: the properties of the homogeneous electron gas are profoundly modified by the emergence of novel physical behaviors that are commonly associated with electrons in atoms, such as the presence of a shell structure in the energy to add electrons. Ordered arrays of quantum dots have also been fabricated.

With regard to the spatial structure of the electronic distribution inside a circularly symmetric quantum dot subject to parabolic confinement, ordering takes place in two well separated stages: radial ordering of the electrons into shells occurs first and is followed by orientational ordering through freezing of intershell rotations at very strong coupling. We have carried out an extensive study of ground-state densities and pair distribution functions over broad ranges of coupling strength and electron number. Increasing coupling strength leads to a spin-polarized state exhibiting a main first-neighbor peak in the radial structure in combination with a fluid-like angular distribution.

4 Conclusions

Many advanced academic institutions are increasingly committed to this modern area of the natural sciences and are thus offering living culture and professional training to their graduating students in physics. It may also be expected that, as progress continues, greater awareness of the quantum world will spread into undergraduate education as well as into mathematics and engineering.

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