First-principles many-body theory for ultra-cold atoms

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Abstract. Recent breakthroughs in the creation of ultra-cold atoms in the laboratory have ushered in unprecedented changes in physical science. These enormous changes in the coldest temperatures available in the laboratory mean that many novel experiments are possible. There is unprecedented control and simplicity in these novel systems, meaning that quantum many-body theory is now facing severe challenges in quantitatively understanding these new results. We discuss some of the new experiments and recently developed theoretical techniques required to predict the results obtained.

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INTRODUCTION

What is the coldest temperature in the universe? We now can access laboratory temperatures as cold as 0.5nK[1]. This is a billion times colder than observed anywhere in space. It is unlikely that such temperatures can be found elsewhere in the universe, unless there are physicists living on other planets. If one were to explain this research to a taxi-driver, the question might be: But, what is it good for? Asked similar questions, Franklin and Faraday are both reputed[2] to have said: What is the use of an infant?

Ultra-cold atomic physics is now beyond the stage of a newborn baby, and scientific progress is exceptionally rapid[3]. A breakthrough of this dimension is rare in science. We have reduced the scale of temperature and thermal energy in ultra-cold gases by an unprecedented six orders of magnitude in just 20 years.

The field of ultra-cold atoms is in many ways a new ball-game. There are no complications from crystal lattices or impurities. The underlying Hamiltonian due to inter-atomic forces is well understood. It is actually exceptionally simple indeed. One can even design Hamiltonians, engineered to a given purpose, using external lasers or magnetic fields to tune these systems. It is now feasible to make quantitative tests of quantum predictions for long-standing models of strongly interacting many-body systems.

The chief current areas of rapid progress include the following areas of physics:

- Bose-Einstein condensates[4, 5]
- Atom lasers and interferometers[6]
- Quantum entangled BECs[7]
- Strongly interacting fermions and universality[8]
• Superchemistry: molecular BEC[9]  
• Itinerant quantum ferromagnets[10]

This new science therefore represent an exceptional change not just in energy scales, but in how we approach experiments. There are great prospects for novel tests of quantum mechanics in mesoscopic regimes of massive particles, never previously explored. However, in order to test quantum mechanics, one must understand its predictions. This raises an extremely important question: how can one make first principles, quantitative theoretical predictions for these quantum many-body systems?

It is important to realize that ultra-cold atomic physics is squarely in the domain of quantum many-body physics, despite the relatively large mass of the atoms. The de Broglie wavelength of atomic $^{23}\text{Na}$ at 0.5$nK$ is $\lambda = \frac{h}{\sqrt{\text{mk}_B T}} \approx 50\mu m$. This exceeds atomic dimensions by more than a factor of $10^5$. It is also far greater than interatomic spacing, which is usually less than $1\mu m$ even in extremely dilute gases. No classical description is remotely applicable, so quantum mechanics must be used. The particle numbers are generally in the range of $10^3 - 10^9$, certainly large enough so to qualify as many body theory.

The theoretical difficulties were well-explained by the founder of quantum field theory, P. A. M. Dirac. In a rare burst of loquacity, Dirac celebrated his discovery of the laws of quantum field theory by remarking[11]:

*The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.*

Why is quantum many-body theory so challenging? Even today, exact solutions are unknown except for very special cases!

This is best explained by recalling that classically, Newton’s laws correspond to a $6N$ dimensional ordinary differential equation for $N$ particles. Quantum mechanics is also the equation of motion of a vector in a large space. However, the dimension of quantum Hilbert space scales exponentially rather than linearly. As an example, consider 500,000 atoms and spatial modes, a typical number in an experiment, corresponding to $3 \times 10^6$ classical dimensions. The equivalent number of quantum bits (qubits) from a quantum theory perspective is $10^6$, and the dimension of the Hilbert space, or total number of quantum states, is $10^{300,000}$. The classical number of variables can be stored and integrated on any laptop computer today. The quantum number of variables requires more storage than there are particles in the known universe.

To make things interesting, ultra-cold experiments often involve extremely strong interactions, whose scattering length can also greatly exceed the interatomic spacing[12, 13]. This renders the use of mean field or perturbation theories highly questionable, due to the strong inter-particle correlations. Even more challenging is the fact that these are typically small or mesoscopic systems, completely isolated from any thermal reservoir. The concept of temperature itself becomes questionable. It is only entropy that is well defined, and therefore measurable.

Finally, to add more zest, many of the experiments carried out are intrinsically dynamical, involving large changes in the Hamiltonian[14]. This can drive the many-body system very far from the ground or thermal equilibrium state. Such large excursions
are rarely found in conventional condensed matter systems. Linear response theory is scarcely applicable to these dynamical experiments. True quantum dynamics of this type is an extreme sport. Little is known; and even exactly soluble Hamiltonians are of no help, as we explain below.

One might hope that probabilistic methods, sampling the Hilbert space, would be feasible. There has been a degree of success with finding ground states using Monte Carlo methods. However, dynamical problems involve the quantum phase problem, making early numerical simulations often impractical. In 1982, Nobel Laureate R. P. Feynman even made the following statement[15]: Can physics be probabilistically simulated by a classical computer? The answer is certainly, No!

In this article, we shall take a more positive approach, and discuss four techniques that are proving successful today. These are:

- Exact solutions in 1D[17, 18]
- Infinite order perturbation theory[19, 20]
- High temperature expansions[21]
- Quantum phase-space methods[22, 23]

Along the way, we will explore the current status of Feynman’s question.

**EXACTLY SOLUBLE MODELS**

A theoretical route that is available in certain quantum many-body problems is the Bethe ansatz. This allows the construction of algebraically exact energy eigenstates. Such methods are mainly useful for one-dimensional quantum gases in thermal equilibrium, which can be experimentally studied using optical lattice techniques.

**Bose gases**

The most famous example of this is the one-dimensional interacting Bose gas. At mass $m$ and interaction strength $g$, this is described by the Hamiltonian:

$$\hat{H} = \int dz \left[ \frac{\hbar^2}{2m} \frac{\partial^2 \hat{\Psi}^\dagger}{\partial z^2} \frac{\partial \hat{\Psi}}{\partial z} + \frac{\hbar g}{2} \hat{\Psi}^\dagger \hat{\Psi}^2 \right] \quad (1)$$

A one-dimensional Bose gas is accessible experimentally using optical lattice techniques with ultra-cold bosonic atoms like $^{87}$Rb. Following early work in the 1960’s, the Bethe ansatz allows the free energy to be calculated through the solution of an integral equation[16]. However, the free energy is not directly measurable in these experiments. A better route to test theoretical predictions is to calculate the density correlation function.

This was first carried out for the finite temperature interacting Bose gas in 2002. Using a combination of the Yang-Yang integral equation solution and the Feynman-Hellman
FIGURE 1. Graph of density correlations versus dimensionless coupling and reduced temperature predicted for a one-dimensional Bose gas[17].

theorem, the normalized local density correlation function is[17]:

$$ g^{(2)} = \frac{\langle \Psi^{\dagger 2} \Psi^2 \rangle}{n^2} = \frac{2m}{\hbar^2 N n^2} \left( \frac{\partial F(\gamma, \tau)}{\partial \gamma} \right)_{n, \tau} $$  \hspace{1cm} (2)

Here $n = \langle \Psi^{\dagger} \Psi \rangle$ is the linear particle density of the bosonic quantum field $\Psi$, $N$ the total particle number and and $F$ the free energy. The quantities $\gamma = m |g| \hbar^2 / n$ and $\tau = T / T_d = 2mT / (n\hbar)^2$ are the dimensionless coupling and temperature respectively, at a physical temperature $T$ and degeneracy temperature $T_d$.

Results for the repulsive case with $\gamma > 0$ show a smooth transition from bosonic correlations at high density to fermionic correlations that are antibunched at low density, with a transition at $\gamma \approx 1$ as shown in Fig (1). This long-predicted fermionization transition has now been experimentally observed[24].

**Fermi gases**

Due to the Pauli exclusion principal, to have a one-dimensional Fermi gas with a local interaction requires at least two spin components. This case is also soluble for ground state and thermal equilibrium properties, using the Bethe ansatz. Here an interesting issue is the question of the polarized gas with an attractive interaction, where ordinary BCS pairing is not possible, described by the Hamiltonian below:

$$ \hat{H} = \int dz \left[ \frac{\hbar^2}{2m} \sum_{i=1}^{2} \left( \partial_{z} \hat{\Psi}^{\dagger}_{i} \partial_{z} \hat{\Psi}_{i} - \hbar g \hat{n}_1 \hat{n}_2 + \delta \mu_c (\hat{n}_1 - \hat{n}_2) \right) \right]. $$  \hspace{1cm} (3)

This leads to the possibility of an unconventional FFLO state with an oscillatory order parameter[18]. Solving the relevant integral equations for the ground state leads to a three phase solution, as shown in Fig (2).
The three phases at fixed chemical potential difference are normal (N), superfluid (SF) and polarized superfluid (SF\textsubscript{P}). Here $\gamma$ is defined as in the Bose case, and $\delta \mu_c/\varepsilon_b$ is the dimensionless chemical potential difference scaled to the two fermion bound state energy. Evidence for this behaviour has now been observed via measurements of density distributions in a trapped, one-dimensional Fermi gas\cite{25}.

**INFINITE ORDER PERTURBATION THEORY**

For higher than one dimension, exact solutions for many particles are not known. However, recent progress in experiments have led to the observation of an exceptionally interesting BEC-BCS cross-over phenomenon\cite{12}, where the scattering length is tuned to a molecular resonance in an interacting Fermi gas. In this limit, one finds that the S-wave scattering length becomes infinite, $a \to \infty$. The resulting scale invariant, strongly coupled physics is universal\cite{20}. The physics is independent of the type of fermion or even its density, apart from a scale factor.

While the universal thermodynamics appears remarkably simple, having no free parameters apart from a dimensionless temperature, there is no known exact solution. Conventional BCS theory - as proposed by Eagles, Leggett and others - gives qualitative but not quantitatively correct results\cite{12}. Another approach is to extend mean field theory by including some terms in perturbation theory to infinite order, to account for the strong coupling. So far only leading order terms in a ladder approximation - corresponding to gaussian pair fluctuations (GPF) - can be calculated in this way\cite{19}.

Nevertheless, this rather simple GPF procedure, which extends the earlier NSR above-threshold theory\cite{26} to the superfluid, low-temperature regime, is remarkably accurate in predicting thermodynamic behaviour with no adjustable parameters. This comparison has led to the first evidence of fermionic universality, in which different experiments with distinct Fermi species and experimental conditions all lay on the same graph\cite{20}. Figure (3) shows a comparison of the GPF/NSR theory to four different recently published experiments\cite{27, 28, 29, 30}. The quantities plotted are the measured energy and entropy of the trapped Fermi gas, which experimentalists were able to measure in a model.
FIGURE 3. $E(S)$ of a strongly interacting atomic Fermi gas of either $^6$Li or $^{40}$K atoms compared to a single theoretical curve predicted by the GPF (NSR) theory. Comparisons are made to four different experiments under different conditions, without fitting parameters. The crossed region indicates the superfluid phase.

independent way. Here, $E$ is the total energy of $N$ trapped atoms in a harmonic trap at temperature $T$, while $T_F$ and $E_F$ are the Fermi temperature and energy respectively.

These results show the utility of ultra-cold atomic physics experiments. These are now able to quantitatively test predictions of quantum many-body theories, even in the challenging regime of a strongly correlated, three-dimensional universal Fermi gas[31].

**VIRIAL EXPANSIONS**

It would be better to have an approach without uncontrolled approximations. This can be achieved at temperatures above the superfluid transition - but still in the microKelvin range - through a low density or virial expansion. At high temperatures there is a controllable, small parameter, given by the fugacity $z = \exp(\mu/k_B T) \ll 1$. In principle, all thermodynamic properties of a interacting Fermi gas can be cluster expanded in powers of fugacity[21, 32], even in the strongly interacting limit.

The thermodynamic potential $\Omega$ of a uniform Fermi gas takes the form,

$$\Omega = -V \frac{2k_B T}{\lambda^3} \left[ z + b_2 z^2 + \cdots + b_n z^n + \cdots \right],$$  

where $\lambda \equiv \left[ \frac{2\pi h^2}{m k_B T} \right]^{1/2}$ is the thermal wavelength. In the noninteracting case, indicated by the superscript “1”, one obtains $b_n^{(1)} = (-1)^{n+1}/n^{5/2}$ for the $n$-th virial coefficient, and we define the change due to interactions as: $\Delta b_n = b_n - b_n^{(1)}$. At unitarity, the virial coefficients are temperature independent and are known theoretically to second order: $\Delta b_2 = 1/\sqrt{2}$, with conflicting calculations to third order. In early 2009, we obtained from exact three-body solutions the result[21] $\Delta b_3 = -0.35501298$. Earlier calculations gave $\Delta b_3 \approx 1.06[33]$, which differs both in magnitude and sign.

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A comparison of experimental data to the virial expansion has now been carried out by Nascimbène et al., and published in 2010[30]. This has led to the confirmation of our theoretical prediction of the third virial coefficient: $\Delta b_3 \simeq -0.35 \pm 0.01$, as well as an experimental determination of the fourth virial coefficient $\Delta b_4 \simeq 0.096 \pm 0.015$. This demonstrates, again, the maturity and precision of ultra-cold atomic gas experiments in unambiguously testing theoretical predictions.

The exact solution of the quantum four-body problem needed for this fourth coefficient is yet to be theoretically obtained. In this respect, experiment has now leapfrogged ahead of theory, leaving a new challenge for many-body theorists. Quantum virial expansions can also give reliable high-temperature dynamical predictions, and comparison with experiments is underway.

**PHASE-SPACE REPRESENTATIONS**

None of the techniques described here so far can give an exact treatment of quantum dynamics. For example, using the exact eigenvalues from the Bethe ansatz encounters severe difficulties, because the calculation of exact overlap amplitudes for any initial state is an exponentially complex problem. Even if this approach were feasible, physics experiments typically have non-integrable, higher-dimensional Hamiltonians.

Despite this, an increasing number of many-body experiments are dynamical, with time-varying Hamiltonians. Fortunately, probabilistic sampling can be used in some cases, despite Feynman’s claim of impossibility. The reason is simply that Feynman’s argument was based on the Wigner phase-space expansion, which is not positive-definite, and does not have a probabilistic sampling. However, the argument does not hold in general. There are nonclassical phase-space expansions of the quantum density matrix which can be evolved in time with positive probabilities, the earliest being the positive-P distribution[34]. Such expansions have a generic form as a positive operator expansion:

$$\hat{\rho} = \int P(\bar{\alpha}) \hat{\Lambda}(\bar{\alpha}) d\bar{\alpha},$$

where $\hat{\Lambda}(\bar{\alpha})$ is a complete operator basis in the quantum Hilbert space, while $P(\bar{\alpha})$ is a positive probability used for sampling purposes.

Early applications included the quantum dynamics of solitons in one-dimensional wave-guides, leading to experimentally verified predictions[35]. A recent proof of principle was a multimode quantum dynamical study of two three-dimensional colliding Bose-Einstein condensates[22]. This is a nonclassical extension of the Glauber-Sudarshan P-representation into higher phase-space dimensions, using coherent-state projectors. The distribution is generically positive and scales linearly with the number of modes, having dimension $d = 4M$ for $M$ modes. In the BEC collision example - which had experimental parameters for ultra-cold atom collisions with $^{23}Na$ - there were 150,000 atoms and $2 \times 10^6$ modes.

Results are given in Fig (4), which compares the +P method with a truncated Wigner phase-space approach, in which the distribution is ‘forced’ to remain positive by truncating third-order terms. The +P results indicate a correlated sphere of emitted atom pairs, in general agreement with recent experiments. By comparison, the Wigner results are
unphysical, with negative densities at large momentum. More quantitative comparisons are underway as the experimental atom counting technology is improved.

A similar technique is also possible with fermions[23], and this closely related Gaussian operator basis method is now regarded as the best technique for finding the ground state of the intractable Hubbard model. The resulting theoretical prediction of no long range order[36] repudiates earlier, approximate calculations, and is highly relevant to the question of modeling high-Tc superconductors. Experimental investigations of this are underway, using fermionic atoms trapped in optical lattices.

Another promising approach uses a multi-component variational strategy, although it is computationally challenging. So far, to obtain full convergence, the method is restricted to one dimension[37], although relatively long integration times are feasible.

Current nonclassical phase-space methods have a finite horizon in either time or inverse temperature. After this time, they suffer rapidly growing sampling error, just like the simulation of classical chaos. Yet, neither the expansions nor the time-evolution equations are unique. Improving quantum dynamical algorithms further appears not impossible, possibly via a unification of phase-space and variational approaches.

**CONCLUSION**

Ultra-cold Bose and Fermi gases are now accessible experimentally. There is a great deal of control and precision in current measurements, and technological improvements are ongoing. This has led to breakthrough experiments that test quantum many-body theory as never before. The new science in this frontier of physics has stimulated the rapid development of novel theoretical approaches. Direct tests of theoretical predictions in experiment are occurring, leading to further advances. In the future, we expect to be able to test the foundations of quantum mechanics in hitherto unexplored domains.
REFERENCES