Perspectives of the theory of spin-polarized quantum systems: beyond the standard Boltzmann equation

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The invited talk was given by the author.

Problems and the latest achievements in the theory of spin-polarized quantum systems are briefly discussed. The current agreement with the experimental data is quite good, but the further improvement of the accuracy of theory is hindered by fundamental problems of the kinetic theory. One of the main goals was to go beyond the simplest Boltzmann equation and a rederivation of the improved versions of this equation for different polarized systems with the emphasis on virial, non-local and non-exchange terms. Some specific applications and boundary effects are presented. The basic problem for polarized dense Fermi-liquids is an applicability of the Landau theory to transverse phenomena. For dilute degenerate systems (e.g., low-temperature liquid mixtures of helium isotopes) the problem is how to go beyond the lowest approximations in density/interaction. Most of the attempts in this direction, especially with regard to superfluid transition in helium mixtures are still unconvincing; this transition remains one of the most intriguing problems of (ultra) low-temperature physics.

1. Introduction

The physics of spin-polarized quantum systems has become a rather mature field. Therefore, some of the attitudes and expectations are changing. One should not expect anymore many new striking and puzzling effects. This does not mean that future developments should be dull and routine – on the contrary, the arising problems are very important and intriguing, but the answers become more and more complicated.

Now we are able to give a reasonable theoretical interpretation to most of the experimental data, but the desire to reconcile some quantitative details often encounters more fundamental problems, and demands an understanding and calcuations on the next level of complexity. Below I will try to give a brief review of new theoretical results and to discuss possible approaches to the problems which seem to me to be the most interesting and important.

It would be hopeless to try to review here the whole field. Many results are already summarized in reviews [1] (helium systems), [2] (hydro-

gen), and in Proc. 3-d Int. Conf. Spin-Polarized Quantum Systems [3]. I will restrict myself mostly to the kinetic phenomena, and discuss mainly, but not only, ³He \(^{\)} systems.

Early theoretical achievements for spin-polarized quantum systems were based on different – often heuristic – adaptations of the nearly standard Boltzmann equation. Proper account for quantum identity of particles and noncommutativity of different spin operators resulted, as a straightforward effect, in two major phenomena: the existence of strong molecular field (leading in turn, to spin waves or so-called identical spin rotation effect) and the giant increase of transport coefficients with polarization (a peculiar macroscopic manifestation of the Pauli principle).

Now attention is concentrated on what lies beyond the simplest versions of the Boltzmann equation, and, naturally, the progress is hindered by the uncertainty in the foundations of kinetic theory. The corresponding questions are important from both fundamental and practical points of view: precise experimental techniques allow one to check even tiny theoretical corrections. Therefore, there were several attempts to go beyond the standard approach, and to derive a more accurate version of the Boltzmann kinetic equation. Unfortunately, all the results are so cumbersome that it would be impossible to present here anything except qualitative comments and discussion.

2. Virial corrections

As soon as one goes beyond the simplest Boltzmann equation, the first check would be to reproduce well-known virial/density corrections from this new kinetic equation. One way to do it is to introduce into the Boltzmann equation some phenomenological terms of the proper symmetry with the coefficients from the fit to other data on virial coefficients [4].

A more rigorous and enlightening approach was developed by the Paris group [5]. These authors argue that the so-called Snider equation (see below) is invalid, and that the derivation of the kinetic equation reproducing the Beth-Uhlenbeck [6] second virial correction is rather unlikely on the basis of standard schemes. As an alternative, they suggest a kind of interaction representation (free Wigner transform) for the single-particle distributions in the collision operator, giving the exact description of twobody collisions and shifting the difficulties towards the description of succession of such collisions. The comparison with more conventional approaches is hindered by the use of non-standard variables. The question one still has to answer is to what extent the use of the free Wigner transform is necessary and unavoidable.

3. Non-local effects

When dealing with a Boltzmann equation for dilute gases, one usually assumes the locality of the interaction, leaving only the lowest-order gradient terms in a collision integral. For dilute gases, this approximation works rather well; but, since the kinetic equation for polarized systems contains some additional—and sometimes small—terms, this assumption should be reevaluated. What is more, for polarized systems we are interested in collective or hydrodynamic modes with a k^2 -spectrum; thus, the gradient terms demand a more intense attention, especially for transverse dynamics.

In gases there are three parameters with the dimensionality of length: the interaction radius a, the density $N^{-1/3}$, and the particle's wavelength $\lambda = \hbar/p$ (p is the characteristic momentum). All three initiate different types of gradient expansions. The most dangerous non-local corrections [7] for non-degenerate gases are of the order of $\hbar\Omega/T$, where T is the temperature, $\hbar\Omega$ is the internal molecular field, $\hbar\Omega \sim (\hbar^2/ma^2)(Na^3)\alpha$, m is the mass of particles, α is the degree of spin polarization ($\hbar^2/ma^2 \sim 1$ K). For non-degenerate dilute gases, the ratio $\hbar\Omega/T$ is small, but, nevertheless, any virial expansion may become meaningless if it does not take into account non-local terms.

The non-local contributions to the molecular field are of two different origins. While some terms are of the usual zero-sound type and are easily incorporated heuristically [1, 8] as renormalizations of the molecular field, the others reflect off-shell contributions and are proportional to the derivatives of the T-matrix (vortex function) T(p, p') in the off-shell directions corresponding to non-conserving energy, $|p| \neq |p'|$, i.e., to $(\partial/\partial q)T(p, p+q)$ with $q \to 0$. These terms give an imaginary contribution to the molecular field although they are still linear in the T-matrix (scattering amplitude).

The same approach for degenerate gases, $T \ll T_{\rm F}$, shows that the non-local corrections are of the order of $\hbar\Omega/T_{\rm F} \sim \alpha(N^{1/3}a)$, and are much more important. Without any unexpected cancellations, these non-local (off-shell) terms will forbid all calculations beyond the first order (see section 8). This may be one of the reasons for a discrepancy between experimental results on spin dynamics [9] and calculations [10] of transverse relaxation parameters $\Omega\tau_{\perp}$ [11] (see section 8).

4. A challenge for the Fermi-liquid theory

An extrapolation of the above non-local corrections to higher densities (towards spin-polarized normal Fermi liquids, such as dense ³He ↑) may signal a failure of a simple picture based on the Landau theory. Troubles are associated with the transverse dynamics (dynamics of spin components of distribution perpendicular to the equilibrium direction of magnetization): the validity of the Landau-type description [1, 12] for longitudinal processes is beyond any doubt.

This conclusion is not the first signal of a possible inconsistency in a standard theory for transverse phenomena in polarized Fermi liquids. Some difficulties spotted earlier include [1, 8]:

- (i) possible large imaginary parts i/τ in the spectrum of off-diagonal in spin components of the quasi-particles' distribution;
- (ii) relatively small transverse relaxation time τ_{\perp} ;
- (iii) integration deep into the Fermi spheres, and not only near the Fermi surface, in order to determine a spin-wave spectrum (integrals of the type $\int \dots (n_+ n_-) d^3p$ with the difference of distributions of up and down spins);
- (iv) considerable renormalization of the Fermi-liquid function because of possible gradient terms in Landau's expansion of a single-particle energy in deviations of distribution:

$$\begin{split} \delta \boldsymbol{\varepsilon}(\boldsymbol{p}, \boldsymbol{\sigma}) \\ &= \mathrm{Tr}_{\boldsymbol{\sigma}'} \int \mathrm{d}^{3} p' \left\{ F(\boldsymbol{p}, \boldsymbol{p}', \boldsymbol{\sigma}, \boldsymbol{\sigma}') \right. \\ &+ F_{i}(\boldsymbol{p}, \boldsymbol{p}', \boldsymbol{\sigma}, \boldsymbol{\sigma}') \frac{\partial}{\partial p'_{i}} + F_{ik}(\boldsymbol{p}, \boldsymbol{p}', \boldsymbol{\sigma}, \boldsymbol{\sigma}') \\ &\times \frac{\partial^{2}}{\partial p'_{i} \, \partial p'_{k}} \right\} \delta n(\boldsymbol{p}', \boldsymbol{\sigma}') \,, \end{split}$$

where the new phenomenological functions F_i , F_{ik} , in contrast to the Landau function F, are related not only to the vortex function, but also to its off-shell derivatives, and may be complex. All these problems are interrelated: all are the consequences of conservation laws for off-diagonal states and of non-trivial spin commutators

in addition to Poisson brackets in the expressions for quasi-classical commutators of single-particle variables. All this presents serious circumstantial evidence against the standard Fermi-liquid approach.

The results for non-local effects in polarized degenerate gases quantitatively demonstrate how the effective renormalization of the Fermi-liquid function increases with the increasing density. And, since the off-shell contributions are imaginary, the corresponding corrections make a molecular field complex leading to a possible broadening of spin-wave resonances. Although the results [7] deal only with the corrections to the molecular field (Fermi-liquid function), it is unlikely to change results by a more accurate calculation of relaxation terms arising from the same collision integral.

On the whole, our understanding of the transverse dynamics in highly polarized dense Fermi liquids does not look very encouraging. I see it as one of the major problems for the theory.

5. Non-exchange processes

Usually one assumes an exchange character of ³He interaction in polarized helium systems. However, non-exchange processes, like a magnetic dipole—dipole interaction, may be extremely important even if they are rather weak. Some of the examples are straightforward [1]: longitudinal spin relaxation, dispersion of the sound velocity, coupling of transverse and longitudinal processes, etc.

A general Boltzmann equation for spin-polarized gases with non-exchange interaction is yet to be derived. The results [7] provide a basis for such an equation, and give an expression for a molecular field for non-exchange gases.

The dipole relaxation time T_1 gave a new example of a quantum nature of the systems involved [13]. The usual estimate in gases is $T_1^{-1} \sim (\hbar \beta^2/a^3)^2 t_0^2 N v \sigma$, where t_0 is the duration of collision with cross-section σ , $v \sim (T/m)^{1/2}$ is the velocity of particles with the magnetic moment β . At high temperatures $\sigma \sim a^2$, $t_0 \sim a/v$, and the relaxation time $T_1^{-1} \sim (\hbar \beta^2/a)^2 N/v \sim$

 $(\hbar\beta^2/a)^2 \ N(m/T)^{1/2}$. At lower temperatures, in the domain of quantum gases [1] with large de Broglie wavelengths, $\lambda \sim \hbar/mv \gg a$, the cross-section of p-wave scattering is $\sigma \sim a^2(a/\lambda)^4$, and the collision time is $t_0 \sim \lambda/v$. Then T_1 obtains a different temperature dependence, $T_1^{-1} \sim (\hbar\beta^2/a)^2 \ (N/v)(a/\lambda)^2 \sim (\hbar\beta^2/a)^2 \ N(T/m)^{1/2} \ (am/\hbar)^2$, with an inevitable maximum on the curve $T_1^{-1}(T)$, $T_1^{-1} \sim (\hbar\beta^2/a)^2 \ N(am/\hbar)$, when $\lambda \sim a$ $(T \sim 1 \ K)$. Calculations at high polarizations should be done very cautiously: the coupling of longitudinal and transverse equations [1] hinders the applicability of the Wang Chang–Uhlenbeck approach to kinetic phenomena.

6. Boundary effects

Boundary effects for polarized systems are more complicated than for non-magnetic ones: one should add specific magnetic processes to usual effects of particles, momentum and energy transfer or accommodation. Practical needs also dictate the study of boundary effects in cases of high longitudinal gradients (with large slip effects and large currents through thin boundary layers), and for very dilute systems when the boundary scattering dominates the relaxation.

There are more questions than answers about the boundary depolarization, sticking and scattering [14]. I will mention only three recent developments. One deals with the sticking of hydrogen particles to surfaces coated by helium films [15]. Now we have a basic understanding of the process and know why the sticking coefficient decreases with temperature approximately as 0.3T (T in K).

The second problem concerns stationary situations with large gradients of temperature and/or polarization along the system. Then one should use slip boundary conditions with a 3 × 3 matrix of slip coefficients [16]. The resulting strong boundary flows lead to considerable renormalizations (several percent in some standard experimental configurations) of quasi-equilibrium parameters.

The third concerns the spin dynamics of systems with strong boundary scattering. Despite the dominant character of the boundary effects in dilute (Knudsen) systems, the boundary scattering practically does not influence the spinwave resonances as far as the surface is smooth or has a sufficient coating (like helium coating for H \uparrow) and the adsorption is insignificant [17]. The formation of dense adsorbed layers changes the spectrum because of considerable exchange between bulk and surface particles leading to dispersion of surface relaxation parameters (like in the Leggett–Rice or Lhuillier–Laloe effect), $D_s \rightarrow D_s/(1-i\Omega_s\,\tau_s)$, analogous to the Leggett effect. This may explain experimental data [18] on the spin-wave spectrum in the very dilute H \uparrow .

7. Links with systems of other types

Spin-polarized quantum systems are unique systems, but their uniqueness is associated more with their "quantum" characteristics than with the presence of spin polarization. In this sense, such systems represent only a tiny subdivision of more general types of systems – systems of particles with internal degrees of freedom. In case of arbitrary, non-spin, internal degrees of freedom the role of spin polarization is played by some asymmetry in the particle distribution between internal energy levels. Most of the effects observed in polarized systems must to some extent exist in other ensembles of multistate particles with nearly any non-Abelian group of internal operators.

The quantum theory of dilute gases of multistate particles (e.g., molecular gases) is usually studied on the basis of the quantum Boltzmann equation which is called in this particular case the Waldmann-Snider equation (see review [19]). This equation does not describe the most interesting effects in spin-polarized systems. One drawback was associated with virial corrections and was improved in ref. [5]. Another was caused by an insufficient account of the quantum identity of particles and was corrected in ref. [7].

The generalized Waldmann-Snider kinetic equation clearly demonstrates that all effects in spin-polarized quantum systems represent a more general class of quantum effects in ensembles of arbitrary multistate particles. What is

more, it is always possible to introduce some pseudo-spin variables making this analogy with polarized systems absolutely transparent. Even such specific effects as spin waves have their analog in other systems as a collectivization of transitions between internal states for multistate particles. Such a collectivization takes place because of a strong molecular field proportional to the commutator in internal variables of distribution functions, $\hbar\Omega = \text{Tr}(\hat{P}\hat{T}[\hat{f}_0, \delta\hat{f}])/\text{Tr}(\hat{P}\delta\hat{f}),$ where $\delta \hat{f}$ is a deviation of distribution from the equilibrium \hat{f}_0 , and \hat{P} is a projection operator. Such quantum effects are large (at least noticeable) at low temperatures when the densities of usual gases are extremely low. One may hope to observe such effects for solid-state quasi-particles rather than in molecular gases. For solid-state quasi-particles the molecular field may split a level ω_0 near the extremum Ω_0 of the forbidden zone; this level, in turn, is collectivized with a k^2 -spectrum (F_0 is the proper Fermi-liquid harmonic, Δ is the curvature of the zone near Ω_0 , Ω_1 is the averaged zone width),

$$\omega(k) \simeq \omega_0 \left(1 + k^2 \frac{\int \frac{\mathrm{d}o}{4\pi} \frac{v_F^2(\theta, \varphi) \cos^2\theta}{(\omega_0 - \Omega_0 + F_0\Omega_1)^3}}{\int \frac{\mathrm{d}o}{4\pi} \frac{(\Omega_0 - F_0\Omega_1)}{(\omega_0 - \Omega_0 + F_0\Omega_1)^2}} \right) ,$$

$$\begin{split} &\omega_0 = \varOmega_0 - F_0 \varOmega_1 + \delta \omega \ , \\ &1 + 1/F_0 = \left[\left(\delta \omega + \varOmega_0 \right) \ln \left(1 + \Delta/\delta \omega \right) \right] / \Delta \ . \end{split}$$

8. Some specific results for dilute ³He ↑ and ³He ↑ - ⁴He mixtures

If for dense quantum systems like liquid ³He the lack of detailed decription is justified by obvious fundamental difficulties, one still may count on a much more consistent theory for dilute polarized systems (³He ↑ gas or dilute ³He ↑ -⁴He liquid mixtures). To a large extent this is true, and such a theory exists [1]. However, the further progress is slowed not only by considerable technical problems, but also by some fundamental ones.

In dilute systems the transport calculations are possible with a certain accuracy at all tempera-

tures [1, 11, 20]. The kinetic equation is solved at different temperatures by different techniques: by Abrikosov–Khalatnikov Brooker-Sykes methods for degenerate systems, and by the Chapman-Enskog at high temperatures [1]. Now we know the transport coefficients in the intermediate temperature range too [21]. These variational results coincide exactly with the results of ref. [22] in the degenerate limit, and with the results of ref. [23] in the hightemperature Boltzmann limit. Such a good extrapolation is possible in the main approximation when all these schemes use constants as trial functions in the final state of solving the Boltzmann equation. It would be rather unlikely to have a universal extrapolation scheme beyond the main approximation.

Another result concerns the calculation [10] of the transverse relaxation time introduced in ref. [11] (see also ref. [1]): in degenerate polarized systems, the difference in velocities/energies for spin-up and spin-down particles results in a considerable anisotropy of the spin-diffusion rate in directions along and perpendicular to the direction of magnetization. This is important for interpretation of data on spin dynamics since most of the NMR experiments involve the transverse processes, while the usual theories deal only with the slower longitudinal spin diffusion. The results [1, 10, 11] improved drastically the agreement with experimental data [9, 24] (fig. 1), but did not eliminate all the contradictions. One of the factors influencing the accuracy of calculations is related to considerable non-local effects mentioned above.

The accuracy of calculations for degenerate systems falls very rapidly with increasing concentration. The accuracy is determined by the single dimensionless parameter $p_{\rm F}a/\hbar$ ($p_{\rm F}$ is the Fermi momentum) which describes all the corrections – regardless of the source – to the single-particle spectrum, interaction, retardation effects, etc. For most of the corrections there are – at least in principle – some reliable schemes of accurate calculations or modeling; the complexity of such schemes is only a technical problem. The fundamental problem arises because the density, N, is proportional to $p_{\rm F}^3$, and the same parameter, $p_{\rm F}a/\hbar$, describes also the contributions of three-,

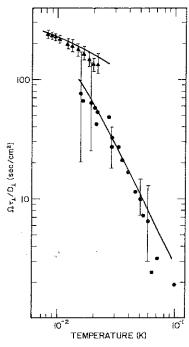


Fig. 1. The temperature dependence of the ratio of the quality factor for spin waves and the transverse spin-diffusion coefficient, $\Omega\tau/D$. The \bullet indicate the experimental data [24] and calculations [1, 11] with the s-wave scattering length a=-0.5 Å (concentration $x=3.7\times10^{-4}$, $T_{\rm F}\simeq13$ mK, H=89 kOe); and the \triangle indicate data [9] with analogous calculations with $a\approx0.77$ Å ($x=1.82\times10^{-3}$, $T_{\rm F}\simeq39.8$ mK, H=80 kOe).

four- and other many-particle interactions and correlations. Since many-body terms cannot be taken into account or reasonably modeled analytically, the more exact calculations involving the single particle spectrum and two-particle interactions lose any sense beyond a certain accuracy in $p_{\rm F}a/\hbar$. Beyond this accuracy the singleparticle spectrum and the interaction potential simply do not exist (instead one should rather operate with a spectrum of Fermi-liquid excitations and a Fermi-liquid function). For all practical reasons, it is senseless to speak about the single-particle spectrum beyond the p^4 -correction, and about the two-particle interaction beyond the first two terms in the s-wave channel. An introduction of any model single-particle spectrum and model interaction potential in order to describe some sets of experimental data

exactly is not very enlightening: such parameterizations are not unique (one can use different forms of parameterization with an equal success) and do not have a reasonable justification; after each new experiment the fitting parameters should be unpredictably adjusted.

On the contrary, the single-particle spectrum and two-body potential for ${}^{3}\text{He}{-}^{3}\text{He}$ interaction in ${}^{3}\text{He}{-}^{4}\text{He}$ mixtures have exact meaning in the Boltzmann region where expansions in interaction, $pa/\hbar \sim \sqrt{(mT)}a/\hbar$, and density, N, are absolutely independent, and many-body corrections may be neglected at low enough concentrations without sacrificing the accuracy of single-and two-particle calculations. Therefore the experiments of the type [24] aimed at measuring the single-particle spectrum are sensible only at high temperatures and low concentrations.

Many of the attempts to model the two-body interaction in degenerate ³He-⁴He mixtures are aimed on an evaluation of a superfluid transition temperature for the ³He subsystem. However, such methods cannot predict reliably even the order of magnitude of T_e: a several percent change in the 'model potential' parameters which do not have direct meaning anyhow and are only some arbitrarily introduced fitting parameters – may change the predicted value of T_{c} by several orders of magnitude. The only prediction [1] with some understandable (but not very high) accuracy is an extrapolation from the low concentrations (where the BCS theory is accurate), providing for T_c at 3% ³He the range between $6 \times 10^{-4} - 2 \times 10^{-2}$ mK which is not very encouraging.

Results [26] prove that even for repulsive s-wave interaction (which is unlikely for 3 He- 4 He), the BCS p-wave pairing is due to the always attractive effective interaction in the p-channel originating from renormalized s-wave processes, rather than to the bare p-wave scattering. This provides additional arguments against the attempts to describe the transition with a conventional p-wave scattering approach. The same general arguments lead to a non-monotonic dependence of T_c on the spin polarization and give a good estimate for T_c since the s-wave pairing is impossible at noticeable polarizations.

Unfortunately, even the most recent experiments do not show any signs of this transition [27], and the question of ³He superfluid transition in ³He-⁴He mixtures remains one of the most intriguing in low-temperature physics.

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