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Thermodynamic aspect in using modified Boltzmann model as an acoustic probe for URu_2Si_2

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ABSTRACT

The approximate system of equations describing ultrasonic attenuation propagating in many electrons of the heavy-fermion materials URu_2Si_2 under high magnetic fields were firstly derived and then calculated based on the modified Boltzmann model considering the microscopic contributions due to electronic fluids. A system of nonlinear partial differential coupled with integral equations were linearized firstly and approximately solved considering the perturbed thermodynamic equilibrium states. Our numerical data were compared with previous measurements using non-dimensional or normalized physical values. The rather good fit of our numerical calculations with experimental measurements confirms our present approach.

1. Introduction

Continuous and discrete kinetic models have been intensively studied (cf. [1]). The thermodynamic equilibrium characteristic for the system investigated using these models is closely related to the constructing invariants (cf. [2]) and the entropy or the H-function for systems considered by kinetic models which represent the entropy with a minus sign [1]. Interpretation of entropy as a thermodynamic potential, which will increase for an isolated system tells us the course of action in other situations [1]. In fact the perturbed state with respect to an equilibrium or a noise [3] may propagate out as an acoustic wave. Thus the thermodynamic aspect of the system could be relevant to the examining of propagation of the plane sound wave or fluctuations (a little away from the equilibrium state) using the kinetic models. Sound propagation in different materials and relevant sound attenuation studies, localization of waves included, have been intensively investigated previously [4,5]. However, most of these papers are using continuum-mechanic approaches [4,5] instead of microscopic models [6–8], such as Boltzmann equations [8]. To describes the collective fluctuations of matter undergoing a phase transition, for instance, to use some magnetic systems to address problems that are central to the broad understanding of strongly correlated materials [9] we need to adopt a microscopic approach. In fact there have been considerable efforts, both experimental and theoretical, as reviewed in Ref. [9], in understanding the heavy-fermion material properties (like U-based intermetallics: URu_2Si_2). Note that near room temperature, these metals have magnetic moments whose magnetic susceptibility suggest that they would order antiferromagnetically at low temperature. However somewhere below certain temperature, unexpected behavior shows up. The electrical resistivity is high for a metal, and the magnetic ordering does not occur. It was as if the rocks in a stream bed began to flow instead of the water. There is still no accepted explanation for such behavior [9].

The heavy fermion metal URu_2Si_2 displays a classic second-order phase transition at T_n = 17.5 K, and yet the nature of the associated order parameter remains elusive nearly two decades after its discovery [10]. The puzzling phase transition at the Neel temperature $T_n \sim$ 17.5 K in the tetragonal heavy-electron (HE) compound URu_2Si_2 is one of the most interesting feature of this material. URu_2Si_2 is a heavy fermion superconductor with a $T_c \sim 1.2$ K and has an antiferromagnetically ordered state with a $T_n \sim 17.5$ K. The superconductivity coexists with the simple antiferromagnetic order oriented along the c-axis of this tetragonal compound. The physical properties of URu_2Si_2 exhibit a strong tetragonal anisotropy also clearly seen in the temperature and field dependence of the elastic constants [11]. For magnetic field: H ∥ c-axis a metamagnetic transition is observed in the field ranging from 35 to 40 T in magnetization measurements [12]. The interesting features at this transition is a three-step process with steps at 35.8, 36.5 and 39.8 T (tesla) at 1.3 K. Despite a large number of investigations, the nature of the intrinsic order parameter of this phase transition has not been identified yet. Interestingly, regarding the phase transition at T_n, the importance of the orbital degree of freedom of the 5f electrons and the instability of the lattice has lately been suggested [13].

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The mysterious phase transition at T_n has features that have both local and itinerant electronic natures, and these coexisting dual characteristics make its description quite challenging. Nevertheless a purely local picture cannot provide a straight-forward explanation for the observed elastic anomalies [11] near T_n that are distinct from those of typical uniaxial antiferromagnets [13] both due to their (weak) magnitudes and due to the absence of precursor effects [14,15] for $T > T_n$. A proper theoretical description of the transition at T_n in URu_2Si_2 must therefore encompass both local and itinerant features of the problem. More specifically, the observed Fermi liquid properties for $T > T_n$ combined with the large entropy loss and the sharp nature of the transition indicate that the underlying quasiparticle excitations are itinerant, presumably composite objects formed from the 5f spin and orbital degrees of freedom of the U ions. Local physics (e.g. Kondo physics, spin-orbit coupling, crystal-field schemes) plays a key role in their development. Some researchers argue that the large entropy loss at the transition can only be understood if the density-wave involves the polarisation of a significant fraction of the quasiparticle band, a condition that discounts a conventional spin-density wave due to the small size of the observed magnetic moment [15].

There is a rich variety of ultrasonic effects in superconducting elements like high temperature superconductors or heavy fermion systems (see e.g. Ref. [16]). In most cases they have not been quantitatively described. In most previous cases of ultrasonic experiments in these compounds we are in the limit $1/kL_e \gg 1$ (k wave number of sound wave, L_e electronic mean free path). Therefore people already noticed pronounced sound velocity effects and only in very rare cases typical sound attenuation effects due to contribution of conduction electrons. Only the field free case H = 0 was treated therein by Lüthi et al. [14].

Meanwhile there was a report that the small but distinct field effects imply that the elastic anomaly in the transverse mode is caused by electrons [17]. In URu_2Si_2, the magnetic fields give rise to a slight but appreciable reduction of the softening in the $(c_{11} - c_{12})/2$ mode. This field dependence suggests that the elastic softening is caused by electrons, in other words, that the observed elastic anomaly is not of the phonon characteristics. They have analyzed the observed data on the two limiting assumptions that the 5f states of URu_2Si_2 are itinerant and well localized [17]. From the former approach based on the simple assumption, they thus suggested the existence of the anisotropic and narrow conduction bands whose degeneracy can be lifted only by the shear strain $\epsilon_{x^2-y^2}$ with the Σ_3 symmetry (of the tetragonal group D_{4h} in this system). In the latter approach, on the other hand, among the proposed crystalline-electric-field (CEF) models [18], the singlet-induced-quadrupolar-ordering model [13] is the best candidate to interpret the observed elastic anomalies. Note that in Ref. [17], the relative change in the elastic constant $\Delta c/c$ was calculated from the relation $c = \rho v^2$, where ρ is the mass density. The ultrasonic measurements are based on the phase comparison method that achieves relative resolution of 2×10^{-6}. The sound velocity v was measured in c_{11}, $(c_{11} - c_{12})/2$ and c_{66} using $LiNbO_3$ plates as ultrasonic transducers.

In this short presentation, based on the modified Blotzmann model or the quantum kinetic approach [19,20], we shall study the weakly damped mode of longitudinal waves in electronic fluids or calculate the ultrasonic attenuation propagating in electronic fluids of the heavy-fermion materials URu_2Si_2 in high magnetic fields considering the contributions due to electronic fluids (which are fermionic fluid). The derived system of equations are highly nonlinear and thus we should firstly use the perturbation method to obtain the linearized (matrix) equations. Our numerical data will be compared with previous measurements [21] using non-dimensional or normalized values. In fact, the rather good fit of our calculations with experimental measurements confirms our present approach.

2. Theoretical formulations

We shall introduce the microscopic approach instead of the continuum mechanic approach below. The modified Boltzmann model such as the continuous Uehling-Uhlenbeck model (or Boltzmann-Nordheim [22], Boltzmann-Uehling-Uhlenbeck (BUU), Uehling-Uhlenbeck (UU) models) [20] reads, in dimensional form [22],

$$\frac{\partial \overline{f}}{\partial t} + \overline{D}(\overline{f}) = \int d\overline{\phi}_1 \int \overline{g}\omega(\widehat{\theta}\overline{g}) d\Omega \left[\overline{f}' \left(1 \pm \frac{\overline{f}}{A^*}\right) \overline{f}_1' \left(1 \pm \frac{\overline{f}_1}{A_1^*}\right) - \overline{f} \left(1 \pm \frac{\overline{f}'}{A^*}\right) \overline{f}_1 \left(1 \pm \frac{\overline{f}_1'}{A_1^*}\right) \right],$$

where the right-hand-side represents the number of particles thrown out of or into the phase element $(\overline{g}\omega(\widehat{\theta}\overline{g})$ satisfying the reversibility which is guaranteed by the Hermitian condition for the transition) [22], $A^* = h^3/(m^3\,\hat{g})$ which, according to the definition of the phase element, is invariant against transformations of the coordinates or momenta (A_1^* included), $\hat{g}$ is the statistical weight of one quantum state, h is the Planck constant,

$$\overline{D}(\overline{f}) = v_x \frac{\partial \overline{f}}{\partial x} + v_y \frac{\partial \overline{f}}{\partial y} + v_z \frac{\partial \overline{f}}{\partial z} + \frac{X}{m} \frac{\partial \overline{f}}{\partial v_x} + \frac{Y}{m} \frac{\partial \overline{f}}{\partial v_y} + \frac{Z}{m} \frac{\partial \overline{f}}{\partial v_z},$$

and m is the mass of the particle, or in dimensionless form,

$$\frac{\partial \widehat{f}}{\partial t} + D(\widehat{f}) = \int d\phi_1 \int g\overline{\omega}(\theta g) d\overline{\Omega} [\widehat{f}'\widehat{f}_1'(1 + \sigma\widehat{f})(1 + \sigma\widehat{f}_1) - \widehat{f}\widehat{f}_1(1 + \sigma\widehat{f}')(1 + \sigma\widehat{f}_1')], \quad (1)$$

where

$$D(\widehat{f}) = \overline{v}_k \frac{\partial \widehat{f}}{\partial \overline{x}_k} + \overline{X}_k \frac{\partial \widehat{f}}{\partial \overline{v}_k}.$$

In above expressions $\overline{v}_k$(e.g., $\overline{v}_x\overline{v}_y\overline{v}_z$) are the three components of the absolute velocity (in coordinate: $\overline{x}_k$ direction), $\overline{X}_k$(e.g., $\overline{XYZ}$) are the three components of the external force per unit mass, and the usual (Einstein) summation convention has been used. The prefactor or function $\overline{\omega}(\theta g)$ $d\overline{\Omega}$ represents the effective cross section for an encounter collision which changes the direction of the relative velocity g of two particles by the angle θ, such that this velocity after collision g' lies within an element of solid angle $d\overline{\Omega} = \sin\theta d\theta d\phi$, where ϕ is the azimuthal angle about g. The subscript 1 denotes functions and variables pertaining to the second particle in the collision, over which the integration takes place, and the primes denote functions and variables which are to be taken after the collision. The differential $d\phi$ reads

$$d\phi = \overline{VG}\left(\frac{m}{h}\right)^3 dv_x dv_y dv_z, \quad (2)$$

where $\overline{G}$ is an eventual weight-factor, and $\overline{V}$ is included for dimensional reasons, but is to be considered as having the value unity to agree with the meaning of $\widehat{f}$ as giving the number of particles per phase cell in coordinate-momenta space of which the space part has unit volume [20]. As already defined in Ref. [20], $\sigma = 0$ is for the Boltzmann statistics, $\sigma = 1$ is for the Bose-Einstein statistics, and $\sigma = -1$ is for the Fermi-Dirac statistics. Moreover $|\sigma|$ can be non-integer (or fractional). This equation has been proved (in either the left-hand or right-hand parts of equation (1)) to be also valid quantum-mechanically (cf. [20] for the details). One possibility is (after changing the dimensions in both sides of equation (1)) $\overline{v}_k \equiv p_k/E$ and $\overline{X}_k \partial/\partial \overline{v}_k \equiv -\nabla_{\overline{x}} U \cdot \nabla_p$, where p_k or the subscript p denotes the momentum, E is the energy, subscript $\overline{x}$ denotes the (spatial) coordinate, and U is the (self-consistent potential or nuclear) mean field. p_k and E can be defined quantum-mechanically after using the Planck constant (thus the uncertainty principle is satisfied [20,23]). Note that in BUU model, following Nordheim [22] to