Quasiparticles and quantum phase transition in universal low-temperature properties of heavy-fermion metals

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received 31 August 2006; accepted in final form 3 October 2006
published online 1 November 2006

PACS. 71.27.+a – Strongly correlated electron systems; heavy fermions.
PACS. 74.20.Fg – BCS theory and its development.
PACS. 74.25.Jb – Electronic structure.

Abstract. – We demonstrate, that the main universal features of the low-temperature experimental \( H-T \) phase diagram of CeCoIn5 and other heavy-fermion metals can be well explained using Landau paradigm of quasiparticles. The main point of our theory is that the above quasiparticles form the so-called fermion-condensate state, achieved by a fermion condensation quantum phase transition (FQPT). When a heavy-fermion liquid undergoes FQPT, the fluctuations accompanying the above quantum critical point are strongly suppressed and cannot destroy the quasiparticles. The comparison of our theoretical results with experimental data on CeCoIn5 have shown that the electronic system of the above substance provides a unique opportunity to study the relationship between quasiparticles properties and non-Fermi–liquid behavior.

Although much theoretical efforts have been devoted to understanding the non-Fermi–liquid (NFL) behavior of heavy-fermion (HF) metals using the concept of quantum critical points, the problem is still far from its complete understanding since the experimental systems display serious discrepancies with the theoretical predictions [1]. A common belief is that a quantum critical point (QCP) is the point where a second-order phase transition occurs at temperature \( T \to 0 \), and where both thermal and quantum fluctuations are present destroying quasiparticles and generating a new regime around the point of instability between two stable phases [2]. Recent experimental studies of the CeCoIn5 HF metal provide valuable information about the NFL behavior near possible QCP due to its excellent tunability by a pressure \( P \) and/or a magnetic field \( H \) [3–6]. The experimental studies have shown that besides a complicated \( H-T \) phase diagram, the normal and superconducting properties around the QCP exhibit various anomalies. One of them is power (in both \( T \) and \( H \)) variation of the resistivity and heat transport [3–8], inherent to both NFL and Landau-Fermi-liquid (LFL) regimes. The
other one is a continuous magnetic-field evolution of a superconductive phase transition from the second order to the first one [9, 10]. The above anomalous power laws can be hardly accounted for within scenarios based on the QCP occurrence with quantum and thermal fluctuations. For example, the divergence of the normal-state thermal-expansion coefficient, $\alpha/T$ is stronger than that in the 3D itinerant spin-density-wave (SDW) theory, but weaker than that in the 2D SDW picture [11]. This brings the question of whether the fluctuations are responsible for the observed behavior, and if they are not, what kind of physics determines the above anomalies? Fortunately, direct observations of quasiparticles in CeCoIn$_5$, CeIrIn$_5$, and Sr$_3$Ru$_2$O$_7$ have been reported recently [4,12,13]. However, if the quasiparticles do exist, why are they not suppressed by the fluctuations? Moreover, these recent facts contradict strongly the theoretical investigations, where quantum phase transitions responsible for the NFL behavior are considered to be of a second kind so that the quasiparticles are inhibited near these phase transitions [1,2].

In this letter we show that these problems can be resolved within Landau quasiparticle picture providing that quasiparticles form the so-called fermion-condensate (FC) state [14] emerging behind the fermion condensation quantum phase transition (FCQPT) [15]. We show that near FCQPT the fluctuations are strongly suppressed while quasiparticles are “protected” from the above fluctuations by the first-order phase transition. We analyze the experimental $H$-$T$ phase diagram of CeCoIn$_5$ and show that its main universal features can be well understood within the theory based on FCQPT. We demonstrate that the electronic system of CeCoIn$_5$ can be shifted from the ordered to disordered side of FCQPT by a magnetic field; therefore giving a unique possibility to study the relationship between quasiparticles and NFL behavior.

To study the low-temperature universal features of HF metals, we use the notion of HF liquid in order to avoid the complications associated with the crystalline anisotropy of solids. This is possible since we consider the (universal) behavior related to the power law divergences of observable variables like the effective mass, thermal-expansion coefficient, etc. These divergences are determined by small (as compared to those from unit cell of a corresponding reciprocal lattice) momenta transfer so that the contribution from larger momenta can be safely ignored. Let us consider HF liquid characterized by the effective mass $M^*$. Upon applying the well-known equation, we can relate $M^*$ to the bare electron mass $M$ [16, 17] $M^* = M/(1 - N_0 F^1(p_F, p_F)/3)$. Here $N_0$ is the density of states of a free electron gas, $p_F$ is Fermi momentum, and $F^1(p_F, p_F)$ is the $p$-wave component of Landau interaction amplitude. Since LFL theory implies the number density in the form $x = p_F^2/3\pi^2$, we can rewrite the amplitude as $F^1(p_F, p_F) = F^1(x)$. When at some $x = x_{FC}, F^1(x)$ achieves some critical value, the denominator tends to zero so that the effective mass diverges at $T = 0$. Beyond the critical point $x_{FC}$ the denominator becomes negative making the effective mass negative. To avoid physically meaningless states with $M^* < 0$, the system undergoes FCQPT with FC formation in the critical point $x = x_{FC}$. Therefore, behind the critical point $x_{FC}$ the quasiparticle spectrum is flat, $\varepsilon(p) = \mu$, in some region $p_i \leq p \leq p_f$ of momenta, while the corresponding occupation number $n_0(p)$ varies continuously from 1 to 0, $0 < n_0(p) < 1$ [14]. Here $\mu$ is a chemical potential. To investigate the FC state at $T = 0$, we apply weak BCS-like interaction with the coupling constant $g$ and see what happens with both the superconducting gap $\Delta$ and the superconducting order parameter $\kappa(p)$ as $g \to 0$. Let us write the usual pair of equations for the Green’s functions $F^+(p, \omega)$ and $G(p, \omega)$ (see, e.g., ref. [16]):

$$F^+ = \frac{-g\Xi^*}{(\omega - E(p) + i0)(\omega + E(p) - i0)}, \quad G = \frac{u^2(p)}{\omega - E(p) + i0} + \frac{v^2(p)}{\omega + E(p) - i0},$$

(1)
where \( E^2(p) = \xi^2(p) + \Delta^2, \) \( \xi(p) = \varepsilon(p) - \mu, \) and the superconducting gap,

\[
\Delta = g|\Xi|, \quad i\Xi = \int \int F^+(p, \omega) \frac{d\omega dp}{(2\pi)^4}.
\]

(2)

Here \( v^2(p) = (1 - \xi(p)/E(p))/2, \) \( v^2(p) + u^2(p) = 1, \) and simple transformations give

\[
\xi(p) = \Delta \frac{1 - 2v^2(p)}{2\kappa(p)}, \quad \frac{\Delta}{E(p)} = 2\kappa(p),
\]

(3)

with \( \kappa(p) = u(p)v(p). \) Next we observe from eqs. (2) and (3) that

\[
i\Xi = \int \int F^+_0(p, \omega) \frac{d\omega dp}{(2\pi)^4} = i \int \kappa(p) \frac{dp}{(2\pi)^3}.
\]

(4)

It follows from eqs. (2), (3) and (4) that when \( g \to 0 \) the superconducting gap \( \Delta \to 0, \)

while \( \xi = 0 \) and the dispersion \( \varepsilon(p) \) becomes flat, providing that \( \kappa(p) \) is finite in some region

\( p_i \leq p \leq p_f, \) making \( \Xi \) finite. Thus, in the state with FC \( \Delta \) can vanish while parameters \( \kappa(p) \)

and \( \Xi \) are finite. Taking into account eqs. (2) and (3) we represent eqs. (1) as follows:

\[
F^+ = -\frac{\kappa(p)}{\omega - E(p) + i0} + \frac{\kappa(p)}{\omega + E(p) - i0}, \quad G = \frac{u^2(p)}{\omega - E(p) + i0} + \frac{v^2(p)}{\omega + E(p) - i0}.
\]

(5)

It is directly seen from eqs. (5) that in the FC state at \( g \to 0, \) the equations for functions \( F^+(p, \omega) \) and \( G(p, \omega) \) take the following form in the region where \( \kappa(p) \neq 0: \)

\[
F^+(p, \omega) = -\kappa(p) \left[ \frac{1}{\omega + i0} - \frac{1}{\omega - i0} \right], \quad G(p, \omega) = \frac{u^2(p)}{\omega + i0} + \frac{v^2(p)}{\omega - i0}.
\]

(6)

Here, the factors \( v^2(p), \) \( u^2(p) = 1 - v^2(p) \) are determined by the condition \( \varepsilon(p) = \mu \) when

\( p_i \leq p \leq p_f. \) Upon integrating \( G(p, \omega) \) over \( \omega \) we obtain that \( v^2(p) = n(p), \) where \( n(p) \) is the quasiparticles distribution function. Taking into account the well-known Landau equation

\[
\delta E[n(p)]/\delta n(p) = \varepsilon(p),
\]

we observe that the equation determining \( n(p) \) takes the form [14]

\[
\frac{\delta E[n(p)]}{\delta n(p)} = \mu, \quad p_i \leq p \leq p_f,
\]

(7)

where \( E[n(p)] \) is Landau functional [16]. Equation (7) describes the state with FC characterized by the superconducting order parameter \( \kappa_0(p) = \sqrt{n_0(p)(1 - n_0(p))}, \) where the functions \( n_0(p) \) are solutions of eq. (7). It is instructive to construct \( F^+(p, \omega) \) and \( G(p, \omega) \) when \( g \) is finite but small so that the functions \( v^2(p) \) and \( \kappa(p) \) can be approximated by the solutions of eq. (7). In that case, \( \Xi, \Delta \) and \( E(p) \) are given by eqs. (4), (2) and (3), respectively. Inserting these into eqs. (5) we obtain the functions \( F^+(p, \omega) \) and \( G(p, \omega). \) It is seen from eq. (2) that \( \Delta \) is a linear function of the coupling constant \( g. \) Since the transition temperature \( T_c \sim \Delta \) tends to zero along with \( g \to 0, \) the order parameter \( \kappa(p) \) of the FC state vanishes at any finite temperature so that at \( T > 0 \) the quasiparticle occupation number is given by the Fermi-Dirac function which we represent in the form \( \varepsilon(p, T) = \mu(T) = T \ln\{(1 - n_0(p, T))/(n_0(p, T))\}. \)

Observing that at \( T \to 0 \) the distribution function satisfies the inequality \( 0 < n_0(p) < 1 \) at \( p_i \leq p \leq p_f, \) we conclude that the logarithm is finite (therefore \( T \ln(\) ...) \( \to 0 \) and again arrive at eq. (7) determining \( n_0(p). \) The entropy \( S[n(p, T)] \) is given by the familiar expression [16]

\[
S[n(p, T)] = -2 \int [n(p, T) \ln n(p, T) + (1 - n(p, T)) \ln(1 - n(p, T))] \frac{dp}{(2\pi)^3}.
\]

(8)
Fig. 1 – \( H-T \) phase diagram of CeCoIn\(_5\). Right panel: the superconducting-normal phase boundary \[10\] is shown by the solid and dashed lines with the solid square showing the point where the superconducting phase transition changes from the second to the first order. The dotted line is given by eq. \( (10) \) and represents the transition \( T^* (H) \) from the Landau-Fermi-liquid (LFL) behavior with the \( T^2 \) regime in \( \rho (T) \) to the \( T^{2/3} \) one. The solid line given by eq. \( (11) \) represents the crossover \( T^* (H) \) from the \( T^{2/3} \) regime in \( \rho (T) \) \[3\] to the non-Fermi–liquid (NFL) behavior with \( \rho (T) \propto T \). Experimental facts obtained from resistivity measurements are shown by the solid squares \[3,4\]. The left panel shows the magnetic-field dependence of \( T^2 \) Landau-Fermi-liquid coefficients of charge \( A(H) \propto (H - H_{c0})^{-4/3} \) and heat \( B(H) \propto (H - H_{c0})^{-4/3} \) transport with experimental data taken from refs. \[3,4\].

It follows from eq. \( (8) \) that the entropy \( S_{NFL} \) related to the special solution \( n_0(p) \) contains the temperature-independent term \( S_0 = S_{NFL}(T \to 0) \sim x(p_F - p_i)/p_F \). Thus, the function \( n_0(p) \) represents the special solutions of both BCS and LFL equations determining the NFL behavior of HF liquid with FC. Namely, contrary to conventional BCS case, the FC solutions are characterized by infinitesimal value of superconducting gap, \( \Delta \to 0 \), while both \( \kappa (p) \) and \( \Xi \) remain finite and \( S = 0 \). In contrast to the standard solutions of the LFL theory, the special ones \( n_0(p) \) are characterized by the entropy \( S \) containing the temperature-independent term \( S_0 \). At \( T \to 0 \) both the normal state of the HF liquid with the finite entropy \( S_0 \) and the BCS state with \( S = 0 \) coexist being separated by the first-order phase transition, where the entropy undergoes a finite jump \( \delta S = S_0 \). Due to the thermodynamic inequality, \( \delta Q \leq T \delta S \), the heat \( \delta Q \) of the transition is equal to zero making the other thermodynamic functions continuous. Thus, both at the FCQPT point and behind it there are no critical fluctuations accompanying second-order phase transitions and suppressing the quasiparticles. As a result, the quasiparticles survive and define the thermodynamic properties of the HF liquid.

On the basis of the above special solutions related to FC, we can explain the main universal properties of the \( H-T \) phase diagram of the HF metal CeCoIn\(_5\) shown in fig. 1. The latter substance is a \( d \)-wave superconductor with \( T_c = 2.3 \) K, while a field tuned QCP with a critical field of \( H_{c0} = 5.1 \) T coincides with \( H_{c2} \), the upper critical field where superconductivity vanishes \[3-5\]. We note that in some cases \( H_{c0} = 0 \). For example, CeRu\(_2\)Si\(_2\) shows no magnetic ordering down to lowest temperatures \[18\]. Therefore, in our simple HF model \( H_{c0} \) can be treated as a fitting parameter. Under the application of magnetic field \( H_{c0} \), CeCoIn\(_5\) demonstrates the NFL behavior down to \( T = 0 \) \[11,19\]. It also follows from the above consideration that \( H_{c0} \approx H_{c2} \) is an accidental coincidence. Indeed, \( H_{c2} \) is determined by \( g \) which in turn is given by the coupling of electrons with magnetic, phonon, etc. excitations rather than by \( H_{c0} \). As a result, under application of a pressure which influences differently \( g \) and \( H_{c0} \), the above coincidence will be removed in agreement with facts \[6\]. At relatively high temperatures, the superconducting-normal phase transition in CeCoIn\(_5\) shown by the solid line in the right panel of fig. 1 is of the second order \[9,10\] and \( S \) and the other thermodynamic quantities
are continuous at the transition temperature $T_c(H)$. Since $H_{c2} \simeq H_{c0}$, upon the application of magnetic field, the HF metal transits to its NFL state down to lowest temperatures as seen from fig. 1. As long as the phase transition is of the second order, the entropy of the superconducting phase $S_{SC}(T)$ coincides with the entropy $S_{NFL}(T)$ of NFL state,

$$S_{SC}(T \to T_c(H)) = S_{NFL}(T \to T_c(H)). \tag{9}$$

Since $S_{SC}(T \to 0) \to 0$, eq. (9) cannot be satisfied at sufficiently low temperatures due to the presence of the temperature-independent term $S_0$. Thus, in accordance with experimental results [9,10], the second-order phase transition converts to first-order one below some temperature $T_0(H)$. To estimate $T_0(H)$, we use the scaling idea of Volovik (see ref. [20] for details), who derived interpolation formula for the entropy of a $d$-wave superconductor in a magnetic field $H$, while $S_{NFL}$ has been estimated in [21]. As a result, upon using eq. (9), we obtain $T_0(H)/T_c \simeq 0.3$. This point coincides pretty well with experimental value, shown in fig. 1. We note that the prediction that the superconducting phase transition may change its order had been made in the early 1960s [22]. Being based on the thermodynamic considerations, our proof is robust and can be expanded to cases when the superconducting phase is replaced by another ordered state. Namely, if the superconducting phase were replaced by some other ordered phase separated from the NFL phase by the second-order phase transition at $H = 0$, then at some temperature $T_0(H)$ this phase transition should change its order. It follows from the above consideration that the NFL phase has the temperature-independent entropy term $S_0$. Since in the ordered phase the Nernst theorem ($S \to 0$ as $T \to 0$) should hold, we conclude that there is the entropy step (from $S_0$ to zero) as $T \to 0$ while a system traverses the phase transition line from the ordered phase to the NFL one. This means that this phase transition should change its order at $T_0(H)$. For example, we predict that the AFM phase transition in YbRh$_2$Si$_2$ with $T_N(H)$ (representing the field dependence of Néel temperature) should become first order at $T \leq T_0(H)$, where $T_0(H)$ is some finite temperature. Under constant entropy (adiabatic) conditions, there should be a temperature step as a magnetic field crosses the above phase boundary due to the above thermodynamic inequality. Indeed, the entropy jump would release the heat, but since $S = \text{const}$ the heat is absorbed, causing the temperature to decrease in order to keep the constant entropy of the NFL state. Note that the minimal jump is given by the temperature-independent term $S_0$, which can be quite large so that the corresponding HF metal can be used as an effective cooler at low temperatures.

The entropy $S_{NFL}$ determines the anomalous behavior of CeCoIn$_5$ in the NFL region of the phase diagram. The term $S_0 \sim x(p_f - p_i)/p_F$ can be determined from the experimental data on spin susceptibility (following Curie law) and the specific heat jump $\Delta C$ at $T_c$ [21]. In HF metals like CeCoIn$_5$ the normalized jump $\Delta C/C_n \simeq 4.5$ is substantially higher than the ordinary BCS value [23], where $C_n$ is the specific heat of a normal state. The specific-heat jump is not proportional to $T_c$ and is related to the fermion condensate parameter $\delta p_{FC} = (p_f - p_i)/p_F \sim S_0/x$, therefore the normalized jump $\Delta C/C_n$ can be large [21,24]. This estimation gives $\delta p_{FC} \simeq 0.044$ [21]. The entropy $S_{NFL}$ determines also both thermal expansion coefficient $\alpha = -\partial S/\partial P$ and Grüneisen ratio $\Gamma = \alpha/C_n$ [21,25,26]. Since the entropy has the temperature-independent part $S_0$, the thermal-expansion coefficient $\alpha \simeq -\delta S_0/\partial P$ becomes temperature independent at low temperatures. Therefore, at $T \to 0$, $\alpha(T) \to \text{const}$, while the specific heat $C_n(T) \to 0$. As a result, $\Gamma(T \to 0)$ diverges in coincidence with the facts [11].

Now we consider the LFL behavior tuned by a magnetic field $H \geq H_{c0}$. The LFL regime is characterized by the temperature dependence of the resistivity, $\rho(T) = \rho_0 + A(H)T^2$, with $\rho_0$ being the temperature-independent part and $A(H)$ is the scattering coefficient. Since the NFL behavior of CeCoIn$_5$ coincides with that of YbRh$_2$(Si$_{0.95}$Ge$_{0.05}$)$_2$ and YbRh$_2$Si$_2$ [27,28]
we would expect that the LFL behavior of these substances also coincide. For example, in YbRh$_2$(Si$_{0.95}$Ge$_{0.05}$)$_2$ the scattering coefficient diverges as $A(H) \propto (H - H_{c0})^{-1}$ [27] while in CeCoIn$_5$ it diverges as $A(H) \propto (H - H_{c0})^{-c}$ with the exponent $c \approx -4/3$ [3–5]. In magnetic fields, the exponent $c = -1$ characterizes the function $A(H)$ of HF liquid with FC [19], while the exponent $c = -4/3$ describes the function $A(H)$ of HF liquid on the disordered side of FCQPT [19, 29, 30]. To understand this striking change in the behavior of CeCoIn$_5$, we recall that FC has just appeared in this substance since $\delta p_{FC} = (p_f - p_b)/p_F \simeq 0.044 \ll 1$. As soon as the magnetic field is sufficiently high, $H \geq H_{c1}$, ($H_{c1}$ is a critical field moving the HF liquid from the ordered side of FCQPT to the disordered side), Zeeman splitting $\delta p_F = (p_{F1} - p_{F2})/p_F$ of the two Fermi surfaces of HF liquid exceeds the condensate parameter, $\delta p_F \geq \delta p_{FC}$, and the HF liquid with FC becomes LFL placed on the disordered side near QCP. Here $p_{F1}$ and $p_{F2}$ are the Fermi momenta of the two Fermi surfaces formed by the application of a magnetic field. The splitting can be estimated as $p_{F}^2 \delta p_F / M^*(H) \sim H \mu_B$, where $\mu_B$ is the Bohr magneton. Taking into account that $A(H) \propto (M^*(H))^{2}$, we obtain $(H_{cr} - H_{c0})/H_{c0} \sim (c_1 \delta p_F)^3$. Our estimations of the coefficient $c_1$ based on the experimental function $A(H)$ show that $c_1 \sim 5$, and we obtain that the reduced field $(H_{cr} - H_{c0})/H_{c0} \sim (c_1 \delta p_F)^3 \approx 0.02$. Thus, we can safely suggest that the reduced field of 0.02 is much smaller than the minimal reduced field 0.1, where $A(H)$ measurements have been carried out in refs. [3, 5]. As a result, the electronic system of CeCoIn$_5$ is placed on the disordered side of FCQPT by the application of such a high field and reveals $A(H) \propto (H - H_{c0})^{-4/3}$. We can see from the left panel of fig. 1 that the coefficient $B(H)$ has the same critical field dependence. Here $B(H)$ stands for the $T^2$-dependent contribution to the thermal resistivity and is related to $A(H)$ by a field-independent factor, $A(H)/B(H) \approx 0.47$, as it should be in the case of ordinary metals [3, 4] and HF metals demonstrating the LFL behavior. At sufficiently low temperatures and decreasing field when $H < H_{cr}$, we predict that CeCoIn$_5$ demonstrates the LFL behavior while the exponent $c$ will change from $c = -4/3$ to $c = -1$.

At low temperatures and $H \sim H_{cr}$, the system remains in the LFL regime, but at elevated temperatures there exists a temperature $T^*(H)$ where the influence of FC related to $S_0$ is recovered and the NFL behavior is restored. To calculate the function $T^*(H)$, we note that the effective mass $M^*$ cannot be changed at $T^*(H)$. Since at $T > T^*(H)$ the effective mass $M^*(T) \propto 1/T$ [31] and at $T < T^*(H)$, $M^*(H) \propto (H - H_{c0})^{-2/3}$, we have

$$T^*(H) \propto (H - H_{c0})^{2/3}. \tag{10}$$

The function $T^*(H)$ given by eq. (10) is represented by the dotted line in the right panel of fig. 1. In high magnetic fields, $H \gg H_{cr}$, there is a new crossover line because the effective mass starts to depend on temperature as $M^*(T) \propto T^{-2/3}$ [29, 30] and $T^*(H)$ becomes

$$T^*(H) \propto (H - H_{c0}). \tag{11}$$

The crossover line given by eq. (11) is represented by the solid line in fig. 1 (right panel). As is seen from fig. 1, the behavior of these lines described by eqs. (10) and (11) is in good agreement with experimental facts [3, 4]. Eventually, when $T_f > T > T^*(H)$ the influence of FC determined by $S_0$ restores and the system demonstrates the NFL behavior with $M^* \propto 1/T$ and $\rho(T) \propto T$ [19, 30]. Here $T_f$ is the temperature at which the influence of FC vanishes. For example, it can be expected by using the condition, $S_0 \ll S(T_f)$. The NFL behavior related to the $S_0$ term can also be observed in measurements of tunneling conductivity and dynamic conductance which are expected to be noticeably asymmetrical with respect to the change of voltage bias from $V$ to $-V$ in HF liquid with FC [32]. Such asymmetrical conductivity was recently observed experimentally in CeCoIn$_5$ [33]. The behavior of the conductivity can be specific when the HF metal transits from its LFL state induced by the application of magnetic
field to NFL one at elevated $T$. We predict that in the case of CeCoIn$_5$ the conductivity being symmetrical in the LFL regime becomes gradually asymmetrical reaching its maximum in the NFL state at elevated temperatures when $T > T^*(H)$ and eventually vanishes.

In summary, we have presented for the first time a theoretical description of the whole phase diagram of CeCoIn$_5$ including the change of the second-order superconducting phase transition to the first-order one under the application of rising magnetic field. We have shown that quasiparticles survive down to lowest temperatures. Our description of the HF metal CeCoIn$_5$ based on the notion of quasiparticles and FCQPT is in good agreement with facts.

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We thank P. Coleman for stimulating discussions. This work was supported in part by RFBR, project No. 05-02-16085. The visit of VRS to Clark Atlanta University has been supported by NSF through a grant to CTSPS.

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