

Properties of electron-hole liquid in highly stressed silicon

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Two independent studies of the electron-hole liquid in stressed Si have provided different values for the ground-state density and the critical temperature of this important Fermi fluid. One set of experiments (by Gourley and Wolfe) was performed using the strain-well configuration while the other (by Forchel *et al.*) employed uniform strain. These differences raise questions of whether there was some basic difference between the two experimental systems or whether the discrepancies lay in the different methods used for data analysis. In the present joint paper these differences are discussed, several aspects of the data are reanalyzed, some new results are presented, and to a large degree the previous differences are removed. In order to test for possible differences between the line-shape analyses, we use the detailed fitting procedure of Forchel *et al.* on the strain-well data of Gourley and Wolfe and thereby find a ground-state density of $(3.7 \pm 0.2) \times 10^{17} \text{ cm}^{-3}$ in the high-stress limit. This ground-state density is found to be close to that originally reported for these data using a simpler analysis. We now believe that the differences in the value of ground-state density arose primarily from differences in the value of the stress used for the high-stress limit; densities derived at the same stress are in agreement. In addition, we now believe that the critical temperature which was reported previously for the strain-confined liquid was overestimated due to compression effects at high excitation levels. By analyzing the dependence of the luminescence spectra on excitation power we estimate the critical point of the strain-confined liquid to be at a lattice temperature of approximately 10.5 K. When account is taken of the possible difference between the lattice and electronic temperatures this value is consistent with the critical temperature of 14 K reported for the uniform-strain case. Finally, a previous anomaly in the data for the phase diagram of the strain-confined liquid is removed; at intermediate excitation levels the density of the liquid is found to be temperature dependent, which is consistent with theory.

INTRODUCTION

Luminescence studies of electron-hole liquids (EHL's) in indirect-gap semiconductors have been of considerable interest because they permit the quantitative evaluation of the ground-state and thermodynamic properties of interacting electronic systems.¹ These properties are of importance for detailed comparison with the results of microscopic many-body theories for the electron gas.² The study of Si in the limit of large stress along the $\langle 100 \rangle$ direction has been of particular importance because in this case the band structure simplifies to a single ellipsoidal hole band and two degenerate ellipsoidal electron valleys. This system is conventionally denoted by Si[2;1]. The rel-

ative simplicity of the band structure in this case makes especially detailed calculations of the correlation energies possible.

In two recent photoluminescence studies,^{3,4} the most extensive and detailed investigations of the properties of EHL's in uniaxially stressed Si were reported. However, there were several differences between the values for key EHL parameters which were determined in these two studies. Forchel *et al.*³ studied the systematic changes in EHL parameters for different band structures. They measured the complete phase diagrams for unstressed Si and for Si stressed along three different axial directions ($\langle 111 \rangle$, $\langle 110 \rangle$, and $\langle 100 \rangle$). From these systematic studies they found that the ratios of measured ground-state

and critical parameters were in agreement with the scaling relations for these quantities proposed by Reinecke and Ying.⁵ In the case of stress σ along $\langle 100 \rangle$ they used $\sigma = 3.7$ kbar and reported a ground-state density for EHL of $n_0 = (4.75 \pm 0.1) \times 10^{17} \text{ cm}^{-3}$ and a critical temperature $T_c = 14.0 \pm 0.5$ K. (1 kbar = 9.8 kgf/mm².) These values agree with ground-state properties calculated using the correlation energies of Vashishta *et al.*⁶ and with critical points calculated using the droplet-fluctuation approach of Reinecke *et al.*⁷ Using a strain-well configuration, Gourley and Wolfe⁴ were able to obtain much higher stresses—up to 16 kbar along $\langle 100 \rangle$. They examined both the variation of the ground-state density and of the EHL lifetime with stress. Based on the theoretical stress dependence of the band structure and the saturation of values obtained for the liquid density with increasing stress, they argued that their highest stresses were well into the infinite-stress limit where the effective masses no longer have a stress dependence. For large stresses along $\langle 100 \rangle$ they reported a ground-state density of $n_0 = 3.5 \times 10^{17} \text{ cm}^{-3}$ and an estimate of the critical temperature of $T_c \approx 20$ K.

It becomes important to understand whether the significant differences reported for the ground-state density and for the critical temperature in these two studies arise from the different methods of photoluminescence-line-shape analysis employed or from the different stress values used, or whether there are intrinsic differences between the EHL system in a strain well as compared to that in the uniform-strain case. In the present joint work we address these questions, and to a large degree, we resolve these differences.

GROUND-STATE DENSITY

In both of these studies the ground-state densities were obtained by fitting the EHL luminescence line shape using a convolution of the electron and hole densities of states and finite-temperature Fermi functions. Quantitative results for the ground-state densities may depend on the inclusion in these fits of a number of detailed features of these systems. Among these features are the effects of intravalley carrier scattering, the difference between the electronic and lattice temperatures, the stress dependence of the hole-band mass, and many-body corrections to the electron and hole masses. These features were treated in different ways in the two studies.

Gourley and Wolfe fitted their spectra using a theoretical line shape which included the nonparabolicity of the hole band, but they did not include the lifetime broadening of the bands due to intravalley scattering nor did they allow for an electronic temperature different from that of the lattice. In addition, they used a single phonon replica in fitting the lineshape instead of considering both the TO and LO contributions to the emission. Forchel *et al.* included intravalley scattering effects via the Landsberg formulation,⁸ allowed the electronic temperature to be a parameter determined by the fit, and included the contributions of both the LO and TO replicas to the spectra. On the other hand, they used a hole density-of-states mass appropriate for the infinite-stress limit.

In order to investigate whether the effects of intravalley scattering and of an electronic temperature different from

that of the lattice were the source of the difference in the values of the ground-state density reported in the two studies, the high-stress spectrum of Gourley and Wolfe from Fig. 10 of Ref. 4 was fitted using the line-shape-fitting procedure of Forchel *et al.* The result, which is shown as the low-power spectrum in Fig. 1 here, yields a density $n = 3.6 \times 10^{17} \text{ cm}^{-3}$ at an electronic temperature of 4.3 K. These values can be compared to $3.5 \times 10^{17} \text{ cm}^{-3}$ at a lattice temperature of 1.4 K obtained by Gourley and Wolfe using their line-shape-fitting procedure. In addition, direct comparisons were made of the effects of the several differences in the line-shape-fitting procedures. For example, the magnitude of the increase in the ground-state density obtained by including the effects of intravalley scattering was found to be $\sim 10\%$, which is consistent with results obtained in previous work.^{3,9} In particular, fitting the low-power spectrum in Fig. 1 without the effect of intravalley scattering gives $n_0 = 3.2 \times 10^{17} \text{ cm}^{-3}$, as compared to $3.6 \times 10^{17} \text{ cm}^{-3}$ obtained above. Thus, we conclude that the different fitting procedures, although significant, were not the primary source of the differences in the reported ground-state densities.

We therefore consider the differences between the stresses employed in the two studies. For the purposes of their study of the systematic variations of the properties of electron-hole liquid with different band structures, Forchel *et al.* selected for the case of stress along $\langle 100 \rangle$ a stress magnitude of 3.7 kbar. For this direction, Forchel *et al.* studied the critical temperature as a function of stress up to $\sigma = 7$ kbar. They found that T_c changed little above a certain stress magnitude, and by using a scaling relation⁵ between the critical density and ground-state density, they argued from the experiment that for stresses ≥ 3 kbar the band structure was to a good approximation

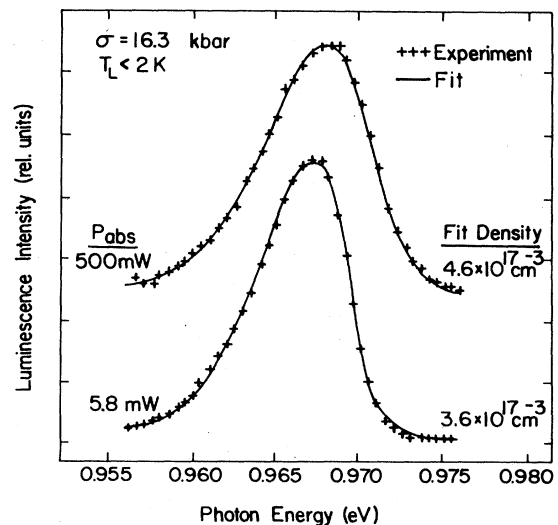


FIG. 1. Luminescence spectra at two different laser powers P_{abs} for EHL in the strain-confined geometry from Gourley and Wolfe, Ref. 4. The fits were made using the procedure of Forchel *et al.*, Ref. 3. T_L gives the lattice temperature and σ the value of the stress.

in the high-stress limit. Using the infinite-stress masses in their line-shape fits they determined the ground-state density to be $4.75 \times 10^{17} \text{ cm}^{-3}$. From calculations of the stress dependences of the masses by Kelso,¹⁰ however, a stress dependence of the hole mass is expected for stresses up to about 10 kbar in the $\langle 100 \rangle$ direction. The effect of using infinite-stress masses in the line-shape fits in this case can be determined by comparison to the data of Wagner, Forchel, and Sauer.¹¹ They examined the changes of electron-hole-liquid properties as a function of increasing stress magnitude. In this study stress-dependent masses were used, and at a stress of 3.7 kbar a ground-state density of $6.0 \times 10^{17} \text{ cm}^{-3}$ was obtained. This value is consistent with that obtained by Gourley and Wolfe for the same stress value.

Therefore, we feel that the largest part of the difference between the reported values for the ground-state density [$4.75 \times 10^{17} \text{ cm}^{-3}$ (Ref. 3) and $3.5 \times 10^{17} \text{ cm}^{-3}$ (Ref. 4)] results from the different magnitudes of the stresses employed in the two experiments. For cases in which the stress magnitudes are similar, the data obtained in the two experiments are in agreement. In the limit of large stress the best value for the ground-state density is estimated to be $n_0 = (3.7 \pm 0.2) \times 10^{17} \text{ cm}^{-3}$. This value corresponds to the value of $3.6 \times 10^{17} \text{ cm}^{-3}$ at 4.3 K extrapolated to zero temperature. At this point, however, it should be noted that a full account has not yet been made for many-body effects on the masses used in the line-shape fits. Theoretical and experimental results for many-body mass enhancements¹² indicate that these effects may increase the densities obtained from line-shape fits by $\sim 15\text{--}20\%$.

This experimental ground-state density $n_0 = 3.7 \times 10^{17} \text{ cm}^{-3}$ is about 20% lower than those calculated^{3,6,7,10} using the most detailed theoretical results⁶ for correlation energy for this system. It should be kept in mind, however, that the EHL ground-state energy and binding energy in Si under large strain is small and that therefore the theoretical ground-state density is sensitive to details of the approximations used in the calculation of the correlation energy. For example, early calculations¹³ of the correlation energy indicated that EHL in Si[2;1] was bound only very weakly if at all. The sensitivity of the theoretical results to details of the calculation also is seen in the recent results of Kirczenow and Singwi,¹⁴ who studied a simplified form of the correlation energy of Vashishta *et al.*⁶ and obtained a ground-state density for Si[2;1] approximately equal to the present experimental result.

CRITICAL TEMPERATURE

We now consider the difference between the reported critical temperatures of 14.0 ± 0.5 K by Forchel *et al.* and 20 K by Gourley and Wolfe for Si with stress along $\langle 100 \rangle$. On general grounds, the value of 20 K seems to be too high. This is because the properties of the EHL are expected to change substantially and systematically with changing band structure in going from unstrained Si to Si[2;1]. This was the case, for example, for the ground-state density discussed above. The value of $T_c = 20$ K

measured by Gourley and Wolfe, however, does not differ in comparable proportion from the value 23.0 ± 1.0 K obtained for Si based on detailed phase-diagram measurements.³ In addition, an unusual feature in the critical-temperature measurement of Gourley and Wolfe was that it was a part of a measured phase diagram which had no temperature dependence for the density on the liquid side. This latter feature is not in agreement with that predicted for a uniform-density Fermi liquid.

Several different procedures have been used to determine experimentally the critical temperature. Forchel *et al.* used two different methods. These were the following: (i) Data for the temperature dependence of the densities on the phase diagrams were fitted with a parametrized form of the droplet-fluctuation model^{7,15} in which the critical temperature is a fittable parameter. In this way the critical point can be located based on data away from T_c for which the gas and liquid luminescence lines do not overlap as strongly as they do near T_c . (ii) For increasing T in indirect-gap semiconductors there is a pronounced shift to higher energies of the low-energy side of the spectra due to the decrease of the liquid density and then to the disappearance of the EHL component. This shift is most pronounced in a narrow region of ≈ 1 K near T_c and has been discussed in detail for the case of Ge.¹⁶ Forchel *et al.* found that these two methods gave consistent results for T_c in the several systems which they studied involving strains in various axial directions, and they found that the results were in agreement with microscopic calculations for these systems. For stress along the $\langle 100 \rangle$ direction the value of T_c was found to be 14 K based on measurements up to 7 kbar.

Gourley and Wolfe determined T_c from a method used by Shah *et al.*¹⁷ for unstrained Si. In this method the position of the low-energy edge of the lowest-energy spectral feature is studied as a function of laser power and temperature. Gourley and Wolfe found that as the power was raised for temperatures below 20 K a regime could be reached where the low-energy edge of the luminescence stopped changing with power. They used this insensitivity of the spectral position as evidence for a constant-density liquid. The position of the low-energy edge, i.e., the renormalized band gap, is related directly to the EHL pair density.^{1,2}

Forchel *et al.*,^{3,18} however, have pointed out that this method is subject to uncertainty because it does not consider the detailed origin of the contributions to the luminescence for the entire line shape. It has been found that the shape of the EHL band just below T_c is similar to that of electron-hole plasma above T_c . They have shown that this method has led to an overestimate of T_c in the past.¹⁹

Recently, an extensive study of the phase diagram of strain-confined EHL's in Ge has been performed by Schowalter *et al.*²⁰ In it, a modified method was used to estimate T_c for the strain-confined droplet of EHL in Ge. This method was also based on the behavior of the low-energy edge of the EHL line with laser power, but a different criterion was used to determine the presence of liquid. The criterion was based on the insensitivity of the position of the luminescence band for decreasing excita-

tion power. For temperatures below T_c the EHL density is fixed by the phase boundary, and it should be relatively insensitive to laser power even at intermediate excitation levels. For Ge it was found that there was a pronounced qualitative change in the power dependence of the spectra at a well-defined temperature (4.5 K). Below this temperature the position of the low-energy luminescence line was stable with power, indicative of an EHL. Above this temperature, the low-energy luminescence line shifted markedly with power, indicative of a variable-density electron-hole plasma (EHP). Thus, the critical temperature of the strain-confined liquid in Ge was estimated to be about 4.5 K.

Figure 2(a) shows a similar effect for strain-confined

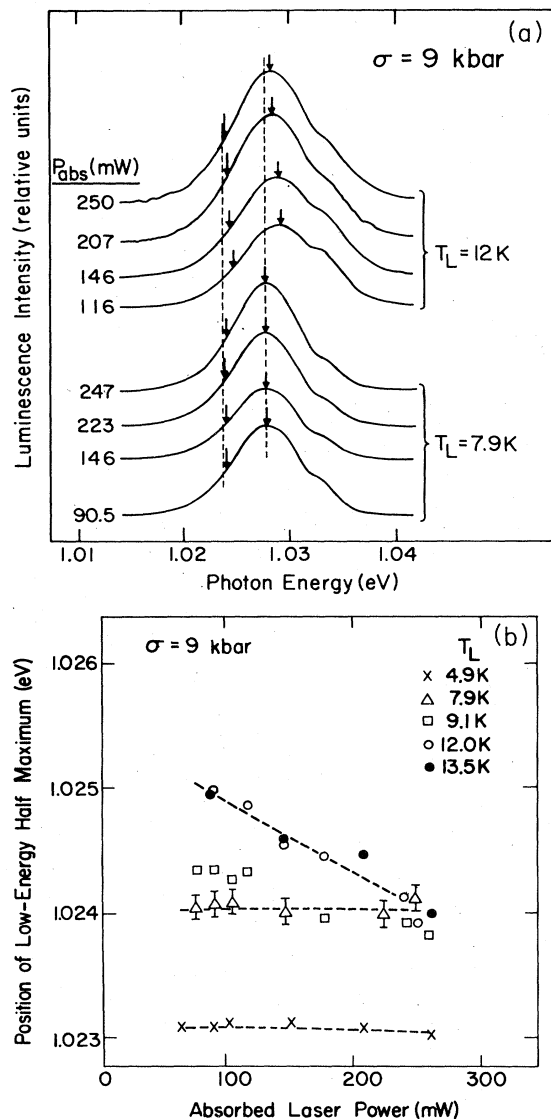


FIG. 2. (a) Luminescence spectra as functions of laser power for lattice temperatures of 7.9 and 12 K. The arrows indicate the positions of the maxima and low-energy half maxima of the lines. (b) The position of the low-energy half maximum of the electron-hole liquid or plasma luminescence line as a function of laser power for several temperatures.

carriers in Si. These data are a previously unpublished subset of the original data of Gourley and Wolfe, and they correspond to a temperature region between that shown in their Figs. 20 and 21 (Ref. 4). We see that at 7.9 K the luminescence-line position is relatively insensitive to power and that at 12 K it is sensitive to power. We suggest that the change in density with power at 12 K is associated with the compressibility of the plasma.

Figure 2(b) is a plot of the low-energy half-intensity position at several different temperatures. Below a lattice temperature of ~ 8 K the spectral position does not shift with power, a behavior which we associate with the presence of the EHL. At 9.1 K the low-energy edge is insensitive to power at low powers but shifts downward at higher powers. We believe this indicates that the EHL is starting to compress at higher excitation levels, and we suggest that such an increased compressibility is associated with temperatures approaching the critical point. The range of powers in these experiments was far above the threshold for EHL formation, so that the low-energy edge of the spectrum was determined by EHL or plasma luminescence and not by that of biexcitons. For $T = 12.0$ and 13.5 K the rate of change of position with power becomes approximately constant. Our interpretation of these data is that for lattice temperature $T < 8$ K the system is well below T_c , for $T = 9.1$ K the temperature is approaching T_c , and the liquid is becoming more compressible, and finally for $T \geq 12$ K the system is above T_c in a plasma state where power changes the density in a way which does not depend strongly on temperature. These data then suggest that the critical point occurs at a lattice temperature between 9.1 and 12 K, to which we assign the value 10.5 K. This value is not expected to change significantly for stresses above 9 kbar, as the ground-state density is virtually constant above this stress.⁴

We feel that the present estimate of the critical temperature at a lattice temperature of ~ 10.5 K in the strain-well case is consistent with the result of Forchel *et al.*, who gave $T_c = 14.0 \pm 0.5$ K. We believe that the difference between these two values may be attributed to the following factors. First, the value in the strain-well case corresponds to a measured lattice temperature, and the electronic temperature is expected to be higher. In the case of the low-power spectrum in Fig. 1, for which a detailed fit has been made above, the difference between the lattice and electronic temperatures was found to be ≈ 3 K. Secondly, T_c may be different due to the different values of the stress in the two experiments. The magnitude of this difference can be estimated from a scaling relation between the critical temperature and the ground state density.⁵ The difference in T_c corresponding to the different ground-state densities is found in this way to be ≈ 1.4 K.

Microscopic calculations using the droplet-fluctuation approach^{3,6} give $T_c = 14.2$ K for Si[2;1]. This is close to the result of Singwi and Tosi,²¹ who obtained 13.8 K using a related method. These results are in agreement with the above experiments. They are, however, lower than the results [17.7 K (Ref. 7), 18.3–24.4 K (Ref. 10), 17.9 K, (Ref. 22), and 20–24 K (Ref. 23)] of other calculations which were based on the uniform-plasma approach. Reinecke *et al.*⁷ have pointed out that this difference is

expected because fluctuations are neglected in these latter approaches.

We can use the present estimate of $T_c = 10.5$ K, which is based on a lattice temperature, to evaluate the ratios in the scaling relations between the ground-state parameters and the critical point as proposed by Reinecke and Ying.⁵ Using, for Si(100), $n_0 = 3.7 \times 10^{17} \text{ cm}^{-3}$ obtained here and $E_x = E_0 + \phi$ with $\phi = 1$ meV the condensation energy,⁴ we find

$$|E_0|/k_B T_c = 15.3, \quad (1a)$$

$$(\kappa T_c / n_0^{1/4})(\kappa / \mu_0)^{1/4} = 1.5 \times 10^{-2} \text{ K cm}^{3/4}. \quad (1b)$$

The values of these ratios predicted theoretically^{5,7} and obtained in recent experiments^{3,16} are ≈ 12 and $\approx 1.8 \times 10^{-2} \text{ K cm}^{3/4}$ for (1a) and (1b), respectively. These ratios depend strongly on the value of T_c , but are weakly dependent on the values of n_0 and ϕ . If we choose a value of T_c for the electronic system $T_c \approx 13\text{--}14$ K, these ratios then are in good accord with both theoretical predictions^{5,7} and with recent experiments.^{3,16} This supports the view discussed above that T_c for the electronic system in Si(100) should be $\approx 3\text{--}4$ K higher than the value of $T_c \approx 10.5$ K based on a lattice temperature.

Finally, we consider the fact that Gourley and Wolfe observed that the density on the liquid side of the phase diagram for the strain well was approximately temperature independent. This is inconsistent with the properties of a Fermi liquid. We feel that this behavior also results from the effects of compression of the EHL and of the plasma at the relatively high excitation powers used. Such compression effects can be seen even at low temperatures.²⁴ Figure 1 shows data taken by Gourley and Wolfe which give EHL spectra at two laser powers in the steepest strain-well configuration that they used. The density increases from $3.6 \times 10^{17} \text{ cm}^{-3}$ at 5.8 mW to an average density of $4.6 \times 10^{17} \text{ cm}^{-3}$ at 500 mW. For all temperatures up to ~ 20 K Gourley and Wolfe observed that the low-energy edge of the liquid spectrum was pushed to approximately the same limiting energy by increasing laser power up to the maximum power that they used. On this basis they concluded that the EHL critical temperature was ~ 20 K and that the EHL density was almost independent of temperature. These features, however, also may be due to the effects of compression. Although both EHL and EHP are compressible, we suggest that at moderate temperatures it is difficult to compress them beyond the zero-temperature EHL density n_0 due to a rapid increase in the system's internal energy. This is consistent with their observation that by increasing laser power (i.e., liquid volume) it was possible to increase the density in the strain well up to n_0 , almost independent of temperature. For temperatures above ~ 20 K Gourley and Wolfe observed that the density at the highest laser power used was lower than n_0 . This behavior may be ascribed to the fact that for these temperatures they may have used insufficient power to compress the plasma to a density $\sim n_0$. Therefore the effects of compression in the strain-well geometry may have precluded Gourley and

Wolfe from observing the characteristic expansion of the EHL and may have given rise to an estimate of a "critical temperature" that was dependent on the strain-well pressure.

We note that the lower-power data for $T \leq 12$ K in Fig. 2 in fact show the low-energy edge of the EHL line moving to higher energy (lower density) for increasing temperature, as expected for a Fermi liquid. Therefore, the phase diagram for the strain-confined EHL at low laser power, where the effects of compression are least important, has a density which decreases with increasing temperature. A decreasing density with increasing temperature is a feature which is expected for a uniform Fermi liquid. In Fig. 2(b) the effect of laser power is greater for temperatures approaching T_c , which is consistent with the compressibility of the system increasing as T approaches T_c .

In conclusion, we have reexamined existing data for the properties of the electron-hole liquid in stressed Si from experiments performed in the strain-well geometry and in the uniform-strain case, and we have presented new results based on these data. We have shown that to a large degree these new analyses reconcile previous differences in the values reported for the ground-state density and the critical temperature for Si[2;1]. It has been found that the ground-state density in the high-stress limit is consistent with a value $n_0 = 3.7 \times 10^{17} \text{ cm}^{-3}$. An estimate of the critical point for the strain-well geometry is that it occurs at a lattice temperature of ~ 10.5 K, which we have argued is consistent with the value of $T_c = 14.0$ K reported for the uniform-strain experiments. Finally, a temperature dependence has been observed for the uncompressed-liquid density in the strain-confined case, as is expected theoretically.

The present experimental value for the ground-state density in the high-stress limit for $\langle 100 \rangle$ -stressed Si is not in complete agreement with theoretical results. The experimental uncertainties may account for this difference, but it is also possible that the EHL in this high-stress limit requires some additional theoretical considerations. The electrons and holes in this limit are at a lower effective density ($r_s \approx 1.8$) than is the case for EHL in unstressed Ge or Si and therefore they are more strongly correlated. This makes the Si[2;1] case a particularly interesting system for future experimental and theoretical work.

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