Criterion for the size of the scaling regime for the metal-insulator transition of doped semiconductors

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In the intermediate regime $n_c < n < n_{CB}$ the Fermi level E_F is above the mobility edge at E_c and below the conduction-band edge at E_{CB} in the so-called impurity band. A simple criterion is developed for the crossover density n_{co} dividing the scaling portion from the more classical portion of the intermediate regime. The scaling of the Hall coefficient determines the itinerant electron density, namely, $-1/eR_H = n_i = \lambda n_c (n/n_c - 1)^g$. Using the two-component model $n_{loc} + n_i = n$, where $n_i(n)$ is a smooth monotonically increasing function of the doping density n, one obtains a relation between λ and g and obtains $n_{co} = n_c / (1 - g)$. This approach yields an expression for the fraction of localized electrons ($E < E_c$) n_{loc}/n_c for $n_c < n < n_{co}$. These predictions are compared with the Hall, NMR, specific heat, and electron spin susceptibility data. This comparison suggests for weak compensation that $1.6n_c < n_{co} < 2n_c$, while for stronger compensation $n_{co} > 3n_c$.

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It has been known for decades that there are local moments on the metallic side of the metal-insulator transition (MIT), and this fact is consistent with the two-component inhomogeneity model formulated by Mikoshiba¹ to explain specific-heat²⁻⁴ and spin-susceptibility^{5,6} data. In addition, there have also been NMR data^{7,8} that has indicated how the density of itinerant electrons decreased toward zero as n $\rightarrow n_{c+}$. Moreover, CESR linewidth data^{9,10} has provided results on the scaling of the itinerant electron density. Historically, as a function of doping density n the behavior has been described in terms of three regimes (see review by Alexander and Holcomb¹¹): (1) $n < n_c$ where as $T \rightarrow 0$ the electrons are all in localized states; (2) $n > n_{CB}$, where the Fermi level is in the host conduction band; (3) an intermediate regime where $n_c < n < n_{CB}$ and the Fermi level is in the so-called impurity band. n_c has been defined by the Mott criterion $(n_c^{1/3}a^* \approx 0.26)$, where a^* is an effective Bohr radius) and $n_{\rm CB} \approx (16/\pi) n_c$ by the Matsubara-Toyozawa¹² criterion. At the lower end of this intermediate regime the transport is characterized by scaling behavior, which is best documented by the scaling behavior of $\sigma_{dc}(n > n_c, T \rightarrow 0)$. Phillips¹³ has called this scaling regime the X phase or filamentary phase and has assumed the current is carried coherently, not diffusively. Unlike magnetic phase transitions where the critical behavior and critical exponents may only be observed very close to T_c , the breadth of the scaling regime is remarkably large (up to $2n_c$) and the reasons for the large breadth of the scaling regime have not been well understood. Below a simple model is employed to provide a result for the breadth of the scaling regime characterized by a crossover density $n_{co} = n_c / (1 - g)$ where g is the scaling exponent of the itinerant electron density n_i . The simplest interpretation of the $\left[-1/eR_{H}(n,T\rightarrow0)=n_{i}(n,T\rightarrow0)=\lambda n_{c}(n/n_{c})\right]$ Hall data $(-1)^{g}$ yields the scaling exponent g. There is now an extensive body of Hall data for Ge:Sb,¹⁴ Si:As,¹⁵ Si:P,^{16,17} Si:B,¹⁸ and other MIT systems that provide experimental determinations of g and λ . However, the smooth behavior of n_i on both sides of n_{co} also yields a relation between the prefactor λ and g. A comparison of this model's predictions with various experimental data provides significant support for this model.

In the two-component model connected with the secondorder MIT at T=0 there are localized electrons with density $n_{\rm loc}$ below the mobility edge at E_c ($E < E_c$) and itinerant electrons with density n_i above the mobility edge ($E > E_c$). The sum of these two densities must equal the net doping density n ($n=N_D-N_A$ for *n*-type semiconductors), namely $n_{\rm loc}+n_i=n$. The divergence of the Hall coefficient $R_H(T \rightarrow 0)$ as $n \rightarrow n_c+$, where n_c is the critical density for the MIT leads to the notion the itinerant electron density $n_i(n)$ scales to zero as $n \rightarrow n_c+$ and suggests $n_i(n)$ can be represented by $n_i(n)=\lambda n_c(n/n_c-1)^g$, where λ is a constant coefficient and g is the scaling exponent. Of interest here is the density dependence of $n_{\rm loc}(n)$ as n increases above n_c . Let us define $f_{\rm loc}\equiv n_{\rm loc}/n_c$, which will be given by

$$f_{\rm loc}(x) = x + 1 - \lambda(x)^g, \tag{1}$$

where $x = n/n_c - 1$. Physically it is plausible that $f_{loc}(x)$ decreases smoothly and monotonically with x, the reduced density, as x increases. At some value of x, which we denote as $x^* f_{loc}(x)$ will become zero. Physically one must have $f_{loc}(x) \ge 0$ because $n_i \le n$. This behavior can be guaranteed if $f_{\rm loc}(x)$ has a minimum $(df_{\rm loc}/dx=0)$ at $x=x^*$. Note that for $x > x^* f_{loc}(x)$ increases with $x - x^*$, which is unphysical behavior; hence the scaling regime for $n_i(n)$ is limited to 0 $< x < x^*$ and x^* provides a direct measure of the size of the scaling regime. For $x > x^*$ Eq. (1) is no longer valid and n_i = n. In doped semiconductors x^* represents the crossover density $n_{co} [n_{co} = n_c(1 + x^*)]$ between scaling behavior and more classical behavior. $n_c < n < n_{co}$ defines the scaling regime, while $n > n_{co}$ denotes the classical regime, but the Fermi energy E_F is still well below the conduction-band edge $E_{\rm CB}$. The condition $df_{\rm loc}/dx|_{x*}=0$ is equivalent to the condition $dn_i/dn = 1$ at n_{co} , or that there is no slope change in n_i vs n at n_{co} . Contrarily, if there were a kink (slope change) at n_{co} this would imply some change in the physics not typically associated with doped semiconductors. Using $f_{\rm loc}(x^*)=0$ and $df_{\rm loc}/dx|_{x=x^*}=0$, one obtains

$$x^* + 1 - \lambda (x^*)^g = 0,$$
 (2a)



FIG. 1. (a) λ versus g for $K_r = 0$ and $K_r = 0.05$. λ is symmetrical about $g = \frac{1}{2}$ for the former and slightly asymmetrical for the latter. The model yields $\lambda_{\text{max}} = 2$ for $g = \frac{1}{2}$ for $K_r = 0$. (b) x^* vs g for $K_r = 0$ and $K_r = 0.05$. For a particular g, Eq. (3a) gives $x^* \propto 1 - K_r$.

$$1 - g\lambda(x^*)^{g-1} = 0.$$
 (2b)

The solution of Eqs. (2a) and (2b) is straightforward and leads to

$$x^* = (1/g - 1)^{-1},$$
 (3a)

$$(\lambda g)^{1/(1-g)} = (1/g-1)^{-1} = x^*.$$
 (3b)

Equations (3a) and (3b) demonstrate that the singleparameter scaling exponent *g* determines x^* and the constant coefficient λ . Thus, with *g* and λ determined one can calculate $f_{loc}(x)$ for $x < x^*$. Since *g* and λ can both be determined from experimental results of the Hall data, the system is over determined and the experimental values of λ can be compared with the values obtained from *g* with Eq. (3b). However, the principal feature of the analysis is that it provides a potentially reliable calculation of $f_{loc}(x)$ that depends on the single parameter *g*.

The quantity $f_{\rm loc}$ does not have to be zero at x^* because there might be a small fraction of localized electrons that remain localized well above $n_{\rm co}$. These might arise from close donor pairs that are well separated from conducting networks (filaments) formed in the random system. If K_r (a constant) is designated as the residual value of $f_{\rm loc}$ at x^* , Eqs. (2a) and (2b) are still readily solved yielding the results $x^* = (1 - K_r)/(1/g - 1)$ and $(\lambda g)^{1/(1-g)} = (1 - K_r)/(1/g - 1)$ $= x^*$. For $x > x^* f_{\rm loc} = K_r = \text{const}$, but note that $n_{\rm loc}/n$ $= K_r(n_c/n)$ and that $n_{\rm loc}/n$ decreases as 1/n with increasing n for $x > x^*$. Certain experimental data⁴ suggest K_r is small (<0.01) for weakly compensated Si:P.

Figure 1 shows values of x^* and λ versus g in the regime 0 < g < 1. Note that x^* increases with g in a nonlinear fashion and diverges as $g \rightarrow 1$. The known experimental values of g lie in the range 0.34 < g < 0.69. $\lambda(g, K_r = 0)$ is shown as a symmetrical function about $g = \frac{1}{2}$ and slowly decreases on



FIG. 2. $n_{\rm loc}/n$ vs reduced density $n/n_c - 1$ for five values of g, namely $\frac{1}{3}$, $\frac{2}{5}$, $\frac{1}{2}$, $\frac{3}{5}$, and $\frac{2}{3}$ for $K_r=0$. For $K_r>0$ the minimum in $n_{\rm loc}/n$ for $\lambda < \lambda_{\rm max}(K_r)$ moves above zero. These curves are only physically valid for $x < x^* = n_{\rm co}/n_c - 1$.

either side of $g = \frac{1}{2}$. For the range of *g* values shown in experiments 1.86< λ <2. This indicates that in the region of experimental interest λ only varies by about 7%, suggesting it will take accurate experimental results to confirm the prediction for $\lambda(g)$ given in Eq. (3b). It is also worth noting that if the impurities have a valence *Z* other than 1 (as in the $M_x \text{Si}_{1-x}$ and $M_x \text{Ge}_{1-x}$ alloys) one should replace λ by $Z_{\text{eff}}\lambda$, where Z_{eff} is the effective valence of the metallic impurity. Figure 1 also shows $\lambda(g, K_r = 0.05)$, which shows the λ values are reduced and $\lambda(g, K_r = 0.05)$ is no longer symmetrical about $g = \frac{1}{2}$.

 $f_{\rm loc}$ has been calculated for five values of g between $\frac{1}{3}$ and $\frac{2}{3}$, and the results are shown in Fig. 2. The features of the five curves are (1) the minimum at x^* moves to higher values as g is increased, but for $g = \frac{1}{2}$ the minimum is at $x^* = 1$ corresponding to $n_{co} = 2n_c$; (2) as the reduced density $n/n_c - 1$ becomes small $f_{\rm loc}$ heads toward unity, but note that the spread in f_{loc} values at a fixed reduced density can be large; (3) at a fixed value of f_{loc} (i.e., $f_{\text{loc}} = \frac{1}{2}$) the change in reduced density $n/n_c - 1$ with g can be more than an order of magnitude for a factor-of-2 change in g; (4) although the curves $f_{loc}(x-x^*)$ are quadratic near x^* for small enough values of f_{loc} the curves are not symmetrical about x^* (which would be better illustrated on a linear scale). The large sensitivity of $f_{loc}(x)$ to the value of g is not surprising and can be useful for a comparison with certain types of data that yield experimental information on the magnitude of f_{loc} at specific values of $n/n_c > 1$. As we shall discuss below, the value of g determined from the scaling of $1/R_H(T \rightarrow 0)$ in a magnetic field may not yield the same value of g as observed in H=0 experiments. Below we discuss several different experiments and compare the experimental values of f_{loc} with those in Fig. 2. Even for n/n_c significantly larger than 2, there might still be some localized electrons that would persist deeper into the metallic regime. This can be addressed by setting f_{loc} to be a constant K_r at the minimum at x^* instead

of zero. The curves for $f_{loc}(g, K_r)$ will have similar shapes to those in Fig. 2. Just as for the $K_r=0$ case the curves for $f_{loc}(g)$ vs n/n_c-1 are only physically meaningful for $x < x^*$.

 $f_{\rm loc}(g = \frac{1}{2}, \lambda)$ has been calculated for three values of λ (1.95, 2.00, 2.05) to investigate the effects of λ when Eq. (3b) is not satisfied and λ is not uniquely determined by g. The values of $f_{\rm loc}$ at the minimum are 0.05, 0.00, and -0.049, respectively, and the minima are still close to x^* = 1. However, the $\lambda = 2.05$ case yields $f_{\rm loc} = 0$ at x = 0.64, and the slope is finite, indicating for n_i there will be a kink or finite change in the slope of $n_i(n)$ vs n for x < 0.64 and x > 0.64. This illustrates the point that a larger value of λ than that given in Fig. 1(a) can lead to unphysical behavior, while a smaller value of λ than that in Fig. 1(a) leads to a minimum in $f_{\rm loc}(x)$ for $f_{\rm loc} > 0$ and is simulated by a finite value of K_r .

The principal experimental approach for determining the scaling exponent g has been from the divergence of the Hall coefficient. The difficulty with the Hall measurement is the application of a magnetic field that alters the wave functions of the itinerant electrons. The size of the electron wave packets can be estimated from the uncertainty principle. The uncertainty in **k** in the vicinity of \mathbf{k}_F will be of order \mathbf{k}_F = $2\pi/\lambda_{dB}$, leading to a wave-packet size $\Delta x > \lambda_{dB}/2\pi$. For electrons with smaller k values the wave-packet size will be correspondingly larger. However, the magnetic length L_H $=(\hbar c/eH)^{1/2}$ is 81 Å at 10 T and 810 Å at 0.1 T. For adequate Hall voltages it is difficult to go to fields well below 0.1 T. For Si:As one has $\lambda_{dB} = 150$ Å at $2n_c$ and 1500 Å at $n = 1.01n_c$. For magnetic fields in the 0.1–1-T range L_H will be the same order or smaller than the wave-packet size and the itinerant electron wave functions will be affected by the magnetic field. Other MIT systems such as Si:P, Si:B, Ge:As, Ge:Ga with smaller values of n_c will have larger values of λ_{dB} and the problem will be more severe. It is not really possible to avoid this problem for barely metallic samples close to the critical density n_c . The magnetic field case represents a different universality class (unitary), and it is known that the scaling exponent of the dc conductivity s(H)increases in a magnetic field for Si:P (Ref. 19) and Si:B (Ref. 20). It is reasonable to suppose the Hall carrier density exponent g(H) will also be affected by a magnetic field, but this has not yet been documented experimentally even though it has been shown for Si:P and Si:B that the conductivity scaling exponent s(H) increases from $\frac{1}{2}$ to near 1 for large magnetic fields in the 8-T range. However, one can now argue that in H=0 the exponent g should be $\frac{1}{2}$ from various zero field experimental results and from the theoretical prediction of Phillips.²¹

Table I gives the experimental values of g and λ and the calculated values of $\lambda(g)$ and n_{co}/n_c from Eqs. (3b) and (3a), respectively. The overall agreement is satisfactory, but it takes very accurate data and a reliable value of n_c to obtain good agreement. The best agreement is for Si:P,¹⁶ Si:As, and Ge:Sb, but the latter case involves significant compensation ($K \sim 20\%$). However, using the smaller value of n_c reported by Ootuka, Matsuoka, and Kobayashi²² for Ge:Sb improves the agreement for λ considerably. g can be affected significantly by small errors in n_c .²³ Errors in n_c directly affect the

TABLE I. Parameters from Hall data.

	n_c (units of 10^{18})	g	$\lambda(K_r=0)$	λ_{expt}	$n_{\rm co}/n_c$
Si:P ^a	3.52	0.36 ± 0.02	1.92	1.97 ± 0.04	1.56
Si:P ^b	3.52	0.44 ± 0.04	1.984	2.25	1.78
Si:As ^c	8.60	0.35 ± 0.02	1.91	1.93 ± 0.04	1.54
Si:B ^{d,e}	4.06	0.45	1.99	4.0	1.82
	4.22	0.37	1.93		1.59
Ge:Sb ^{f,g}	0.168	0.69 ± 0.1	1.857	1.57	3.22
	0.144			1.83	
^a Reference 16.			^e Reference 23.		
^b Reference 17.			^f Reference 14.		
^c Reference 15.			^g Reference 22.		

^dReference 18.

values of λ_{expt} since $(1/n_c)eR_H(n=2n_c, T\rightarrow 0) = \lambda_{\text{expt}}$. The reasons for the 13% too large value of λ_{expt} for Si:P (Ref. 17) and the 100% too large value for Si:B are unclear. The values of n_{co}/n_c range from 1.55 to 3.2. The large value for Ge:Sb is due to compensation, which implies there will be more localized electrons (and local moments) to larger values of n/n_c , which is clearly demonstrated by the data for Ge:Sb. The Si:P and Si:As data (very weak compensation) show from the Hall data that $n_{co}/n_c > 1.5$ but the data do not extend to large enough n to see the high density result $n_i = n$ (for $K_r=0$). The early extensive data of Yamanouchi, Mizuguchi, and Sasaki²⁴ over a range of 100 in donor density clearly shows this crossover. For $n > 6 \times 10^{18}$ /cm³ $n_i = n$, while n_i drops rapidly below *n* for $n < 4.33 \times 10^{18} / \text{cm}^3$. These densities were determined by RT Hall results (all donors ionized) and $-1/eR_H = n$, neglecting the Hall A factor correction ($A \sim 1.2 - 1.3$ for Si:P with $10^{18} < n < 10^{19}$). Neglecting A yields $2.88 < n_c < 3.12 \times 10^{18}$ /cm³ and suggests that $1.4 < n_{co}/n_c < 2$, which agrees qualitatively with the results in Table I for Si:P. These data were at 4.2 K and will not give a reliable value of n_c , but the results are reliable for $n > 1.3 n_c$ where $E_F - E_c \gg kT$.

The zero magnetic field transport data suggest the diffusivity $D = v_F^2 \tau/3$ scales with an exponent twice that for $\sigma_{\rm dc}(n,T\rightarrow 0) \propto (E_F - E_c)^{1/2}$, which when combined with the Einstein relation $eD = \frac{2}{3}(E_F - E_c)\mu$ suggests μ does not scale. The Boltzmann-Drude result $\sigma_{dc} = n_i e \mu$ then implies that $n_i \propto (n/n_c - 1)^{1/2}$, $g = \frac{1}{2}$, and $n_{co}/n_c = 2$. The scaling of the excess CESR linewidth yields $\Delta H_{pp,ex} \propto 1/\tau_c$ $=N_i v_F \langle \sigma_c \rangle$, where $N_i = n_i$ for no compensation. The experimental results¹⁰ for Si:As lead to g = 0.45 and for Si:P g =0.4, leading to $1.66 < n_{co}/n_c < 1.82$. In the scaling regime $k_F l < 1$ and this quantity scales to zero as $n \rightarrow n_c$. The inequality $l(n) \le d(n) \le \lambda_{dB}(n)$ is obeyed, where l(n) is the mean free path, d(n) is the mean donor spacing, and $\lambda_{dB}(n)$ is the de Broglie wavelength associated with the itinerant electrons. Just above $n_c l(n) \ll \lambda_{dB}(n)$ and the size of the itinerant electron wave packets is very much larger than l(n) $[l(n)=\sqrt{3}(D\tau)^{1/2}]$. Thus, the scaling regime represents diffusive behavior, contrary to the Phillips¹³ assumption of coherent conduction in the filaments.

Before discussing other types of data one should mention a different approach of dividing the intermediate regime into a scaling regime and a metallic regime given by Shlimak et al.²⁵ These authors suggest a scaling region followed by a metallic region with a crossover between the scaling and metallic regions occurring at a value of $\sigma(n \ge n_c, T \le 1 \text{ K})$ $=\sigma_m$, where σ_m is Mott's minimum metallic conductivity. Based on Ge:As data they obtain $n_{co}/n_c \sim 1.27$. From earlier data they suggest a ratio 1.26 for Ge:Sb and 1.08 for Ge:Ga. If this same criterion were applied to Si:P and Si:As one would find ratios of 1.0059 for Si:P and 1.0054 for Si:As. This represents about a factor of 50 in $n/n_c - 1$ for these different systems, which provides no evidence for universality. In all of the systems $\sigma(n \ge n_c, T \rightarrow 0)$ exhibits scaling behavior to much larger values of n/n_c , namely of order 2 for weakly compensated Si:P and Si:As and to even larger values for compensated Ge:Sb.14 The Ge:As data in Fig. 2 in Ref. 25 shows no evidence of deviations from scaling up to $n/n_c \sim 1.6$. However, $\sigma(n > n_c, T \rightarrow 0)$ is not as sensitive a measure of the crossover from scaling as the other measurements discussed herein.

The Si:P specific heat^{3,4} and susceptibility data³ give information on the density of localized moments (note that $n_{\rm LM} < n_{\rm loc}$ since some donor pairs and even clusters with very large exchange coupling J have negligible local moments). Paalanen *et al.*³ estimate $n_{\rm LM}/n = 0.25$ and 0.10 for their $1.09n_c$ and $1.25n_c$ samples when all the electrons are localized for $n \leq n_c$. From Fig. 2 these values would correspond to g in the 0.33–0.37 range if $n_{\rm LM} = n_{\rm loc}$, but with slightly larger values for $n_{\rm LM} < n_{\rm loc}$. From specific-heat measurements (including the Schottky anomaly results in a fixed magnetic field) Lakner and v. Löhneysen⁴ obtain for a sample close to $2n_c n_{\rm LM}/n \sim 0.003$ ($n_{\rm LM}/n_c \sim 0.006$). From Fig. 2 this yields $g \approx \frac{1}{2} + \epsilon$ ($\epsilon < 0.02$). Despite this possibly fortuitous agreement with $g = \frac{1}{2}$ the results in Ref. 4 do not yield a maximum in $n_{\rm LM}$ at n_c but rather in the vicinity of $0.6n_c$. At T=0 the maximum in n_{loc} must occur at n_c . The Quirt and Marko⁵ Si:P spin susceptibility data from ESR measurements shows virtual Pauli behavior for n > 1.3 $\times 10^{19}$ /cm³; however, they report for a 5.9 $\times 10^{18}$ sample $(n/n_c \sim 1.58) n_{\rm LM}/n \sim 0.14$. From Fig. 2 this corresponds to $g \sim 0.57$. However, it should be emphasized the standard

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Pauli susceptibility χ_P for itinerant electrons is valid for $n > n_{\rm co}$, but a modified scaling form must be employed for $n < n_{\rm co}$. These authors used a Curie-Weiss form for the susceptibility of localized electrons rather than the more successful treatment of Bhatt and Lee²⁶ of a wide range of antiferromagnetic Heisenberg $J(R_{ij})$ and $\chi_{\rm loc}(T) \propto T^{-\alpha}$, where α is near 0.6, but some data⁴ suggest a density-dependent $\alpha(n)$. The Si:P electron spin susceptibility data yield 0.35 < g < 0.57.

The NMR data of Brown and Holcomb⁷ for ³¹P show a mean Knight shift $\langle K \rangle$ that increas as *n* decreases toward $2n_c$, and these authors note the lack of evidence for local moments. This is consistent with $n > n_{co}$ for their samples and $K_r \sim 0$. Alloul and Dellouve⁸ performed a particularly interesting ³¹P NMR study spanning the MIT for $0.75n_c$ $< n < 21 n_c$. They observed that $\langle K \rangle$ increased with decreasing *n* down to $1.1n_c$ with no apparent change in behavior near $2n_c$. They also observed a substantial decrease in their ³¹P intensity measured by $x = n_i/n$, namely, the fraction of itinerant electrons. When this is converted to n_i/n_c the comparison with the above two-component model is satisfactory qualitatively, but leads to values of g in the range $\frac{2}{3} < g$ < 0.9, which is too large for weakly compensated Si:P. These measurements are at much larger magnetic fields (H=2 T)and the lowest temperature (T=1.65 K) is not low enough just above n_c where there is a significant T dependence of x(T). In addition x is still less than 1 at $3n_c$ ($f_{loc} \sim 0.39$), which is consistent with significant compensation and a larger values of g.

In summary, the two-component model and smooth variation of $n_i(n)$ through the crossover density $n_{co} = n_c/(1-g)$ yields a relation between the scaling exponent g and the prefactor λ and permits the calculation of $f_{loc}(n) = n_{loc}(n)/n_c$ for $n_c < n < n_{co}$. The comparison of this model with a large body of experimental data, with particularly good agreement for the Si:P and Si:As Hall data, suggests the validity of the model, providing a simple explanation for the large breadth of the scaling regime between n_c and n_{co} . The physical significance is that scaling expressions must be used for physical quantities such as $E_F - E_c$, $1/eR_H$, D, k_F , the mean free path l, the density of states $N(E_F)$, and χ_P in this scaling regime.

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