

FERMI SURFACES OF CRYSTALS IN A HIGH MAGNETIC FIELD

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A method of building and investigation of the Fermi surfaces for three-dimensional crystals subjected to a uniform magnetic field is presented. The Hamiltonian of a charged particle in the crystal is treated in the framework of the zero-range potential theory. The dispersion relation for the Hamiltonian is obtained in an explicit form.

Keywords: Fermi surface; crystal in a high uniform magnetic field.

1. Introduction

The shape of the Fermi surface determines the kinetic and equilibrium properties of the electron gas in the crystal matter¹ as well as the dynamics of a single electron in crystal.² The Fermi surface vary considerably in shape with magnetic field.³ However, a high uniform magnetic field changes drastically the translation properties of an electron in the crystal lattice: the appearance of a new length scale (the magnetic length) leads to the famous phenomena related to the “commensurability–incommensurability” transitions. In particular, a fractal structure arises in the diagram describing the dependence of the two-dimensional electron spectrum on the magnetic flux (Azbel’–Hofstadter butterfly^{4,5}). It was shown recently that this fractal structure is an inherent characteristic not only of two-dimensional spectral diagrams but also of the “flux–energy” and “angle–energy” diagrams for a three-dimensional magneto-Bloch electron^{6,7} (a fractal is by definition a set of which the Hausdorff–Besicovitch dimension strictly exceeds the topological dimension⁸).

The translation symmetry of the Bloch electron in a uniform magnetic field is defined by the magnetic translation group,⁹ which has more complicated structure in comparison with the translation group without the field. In particular, the ordinary quasi-momentum is no longer a conserved quantity, therefore, at high magnetic fields a modification of the definition of the Fermi surface is required. Such

a modification is given by V. Ya. Demikhovskii with coworkers.¹⁰ In Ref. 10, the construction and investigation of the Fermi surfaces in the magnetic Brillouin zone have been performed by means of the tight-binding approximation. In particular, it was shown that the change of the topology of the Fermi surface under the influence of the magnetic field can cause the metal–semiconductor transition.

The procedure of obtaining the tight-binding Schrödinger operator (also called the Harper operator) leads to a rather rough approximation of the initial Hamiltonian; for example, in the 2D case it is known that the “flux–energy” diagram for the original periodic Landau operator differs essentially from the classical Hofstadter butterfly.^{11,12}

In this connection, it is interesting to build and investigate the Fermi surfaces in the magnetic Brillouin zone for the periodic Landau operator without additional approximations. Here we consider the case of the Landau operator perturbed by a lattice Λ of short-range scatterers. To get an explicitly solvable model we deal here with a limiting case of the short-range potential, namely, with the zero-range potential,¹³ also called “point potential” (this method was used earlier for obtaining the Fermi surfaces in 3D crystals without magnetic field¹⁴). On the other hand, the spectral properties of the three-dimensional Landau operator perturbed by a periodic point potential was studied in Refs. 7, 15 and 16. In particular, in Ref. 16, a version of the magneto-Bloch analysis was proposed which makes it possible to get an explicit form of the dispersion relation for the problem we consider here.

2. The Model Hamiltonian and Dispersion Relation

We start with the quantum-mechanical Hamiltonian H_0 of a single electron subject to a uniform magnetic field \mathbf{B}

$$H_0 = \frac{1}{2\mu} \left(\mathbf{p} - \frac{e}{c} \mathbf{A}(\mathbf{r}) \right)^2, \quad (1)$$

where e and μ are the charge and mass of the electron, respectively, and $\mathbf{A}(\mathbf{r})$ is the vector potential of the field \mathbf{B} . We choose the symmetric gauge: $\mathbf{A}(\mathbf{r}) = \mathbf{B} \times \mathbf{r}/2$; in this case the form of H_0 in any Cartesian coordinate system with the z -axis directed along the field \mathbf{B} is independent of the choice of the other coordinate axes.

We use the standard notations $\omega = |eB|/c\mu$ (the cyclotron frequency), $l_M = (\hbar/\mu\omega)^{1/2}$ (the magnetic length), and $\phi_0 = 2\pi\hbar c/|e|$ (the magnetic flux quantum). Throughout the paper we denote by \mathbf{b} , $\mathbf{b} = -\mathbf{B}/\phi_0$, the vector of the magnetic flux density: if \mathbf{a}_1 and \mathbf{a}_2 are nonzero vectors, then $|\mathbf{b}(\mathbf{a}_1 \times \mathbf{a}_2)|$ is the total number of the magnetic flux quanta through the parallelogram spanned by \mathbf{a}_1 and \mathbf{a}_2 . Note that $|\mathbf{b}| = (2\pi l_M^2)^{-1}$.

All important physical information concerning the Hamiltonian H_0 is contained in the Green function G_0 at energy E defined as $G_0(\mathbf{r}, \mathbf{r}'; E) = \langle \mathbf{r} | (E - H_0)^{-1} | \mathbf{r}' \rangle$. It is known (see, e.g., Ref. 17) that this function can be represented in the following

forms:

$$G_0(\mathbf{r}, \mathbf{r}'; E) = \Phi(\mathbf{r}, \mathbf{r}') F_1(\mathbf{r} - \mathbf{r}'; E) = \Phi(\mathbf{r}, \mathbf{r}') F_2(\mathbf{r} - \mathbf{r}'; E), \quad (2)$$

where

$$\Phi(\mathbf{r}, \mathbf{r}') = \frac{\mu}{2^{3/2} \pi \hbar^2 l_M} \exp \left[-\pi i \mathbf{b}(\mathbf{r} \times \mathbf{r}') - \frac{(\mathbf{r}_\perp - \mathbf{r}'_\perp)^2}{4l_M^2} \right], \quad (3)$$

$$F_1(\mathbf{r}; E) = \sum_{l=0}^{\infty} \frac{\exp \left[-\sqrt{2(l+1/2 - E/\hbar\omega)} |\mathbf{r}_\parallel| / l_M \right]}{\sqrt{l+1/2 - E/\hbar\omega}} L_l \left(\frac{\mathbf{r}_\perp^2}{2l_M^2} \right), \quad (4)$$

$$F_2(\mathbf{r}; E) = \int_0^{\infty} \frac{\exp \left[-\left(\mathbf{r}_\perp^2 / (e^t - 1) + \mathbf{r}_\parallel^2 / t \right) / 2l_M^2 \right]}{(1 - e^{-t}) \exp \left[(1/2 - E/\hbar\omega)t \right]} \frac{dt}{\sqrt{\pi t}}. \quad (5)$$

Here \mathbf{r}_\parallel is the projection of \mathbf{r} on the direction of the field \mathbf{B} and $\mathbf{r}_\perp = \mathbf{r} - \mathbf{r}_\parallel$; the function $L_l(x)$ is the l th Laguerre polynomial.

It is convenient to decompose G_0 into a sum of singular and regular (with respect to the limit $\mathbf{r} \rightarrow \mathbf{r}'$) parts:

$$G_0(\mathbf{r}, \mathbf{r}'; E) = \frac{\mu}{2\pi \hbar^2} \frac{\exp \left[-i\pi \mathbf{b}(\mathbf{r} \times \mathbf{r}') \right]}{|\mathbf{r} - \mathbf{r}'|} + G_0^{\text{reg}}(\mathbf{r}, \mathbf{r}'; E). \quad (6)$$

Note that $G_0^{\text{reg}}(\mathbf{r}, \mathbf{r}; E)$ is well defined at $\mathbf{r} = \mathbf{r}'$ and

$$G_0^{\text{reg}}(\mathbf{r}, \mathbf{r}; E) = \frac{\mu}{2^{3/2} \pi \hbar^2 l_M} \zeta \left(\frac{1}{2}, \frac{1}{2} - \frac{E}{\hbar\omega} \right), \quad (7)$$

where $\zeta(s, v)$ is the generalized Riemann zeta-function (in other words, the Hurwitz zeta-function).¹⁸

Now we consider a crystalline lattice Γ with nodes γ ; we denote the Bravais lattice of the crystal by Λ . Choose a basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of Λ , then a basic cell C_Γ of Γ (the Wigner-Seitz cell) is fixed: $C_\Gamma = \{t_1 \mathbf{a}_1 + t_2 \mathbf{a}_2 + t_3 \mathbf{a}_3; 0 \leq t_i < 1\}$. If K is the set of nodes of Γ containing in C_Γ , then $\Gamma = K + \Lambda$; this means that each vector $\gamma \in \Gamma$ can be represented in the form $\gamma = \kappa + \lambda$, where $\kappa \in K, \lambda \in \Lambda$ (note that such a representation is unique). Without loss of generality we will suppose that $\mathbf{0} \in K$. We choose the potential $V(\mathbf{r})$ of the crystalline lattice Γ in the form

$$V(\mathbf{r}) = \sum_{\kappa \in K} \sum_{\lambda \in \Lambda} V_\kappa(\mathbf{r} - \lambda), \quad (8)$$

where $V_\kappa(\mathbf{r})$ is the confinement potential near the node κ . To obtain an explicitly solvable model, we pass to the zero-range limit for V_κ . This means that we consider V_κ as the limit of potentials of the form $c_\kappa W(\mathbf{r} - \kappa)$, where $W(\mathbf{r}) \sim 0$ outside a small sphere of radius R centered at zero, the coupling constant c_κ is of order R , and $\int W(\mathbf{r}) d\mathbf{r} = 1$. At the limit $R \rightarrow 0$ the potential V_κ is characterized by one

parameter only, namely, by the scattering length ρ_κ , which is related to the binding energy of the ground state for V_κ by¹³

$$E_\kappa = -\frac{\hbar^2}{2\mu\rho_\kappa^2}.$$

What is important, at the zero-range limit, is the Green function $G(\mathbf{r}, \mathbf{r}'; E)$ of H has the following explicit expression in terms of the Green function $G_0(\mathbf{r}, \mathbf{r}'; E)$ of H_0 (see Refs. 15 and 16):

$$G(\mathbf{r}, \mathbf{r}'; E) = G_0(\mathbf{r}, \mathbf{r}'; E) - \sum_{\gamma, \gamma' \in \Gamma} G_0(\mathbf{r}, \gamma; E) (S^{-1}(E))_{\gamma, \gamma'} G_0(\gamma', \mathbf{r}'; E), \quad (9)$$

where $S^{-1}(E)$ is the matrix inverse to the infinite matrix $S(E)$ with elements

$$S(\gamma, \gamma'; E) = \left[G_0^{\text{reg}}(\gamma, \gamma'; E) - \frac{\mu}{2\pi\hbar^2\rho_\gamma} \right] \delta_{\gamma, \gamma'} + (1 - \delta_{\gamma, \gamma'}) G_0(\gamma, \gamma'; E). \quad (10)$$

The Hamiltonian $H = H_0 + V$ in some sense is a three-dimensional analogue of the one-dimensional Kronig–Penney Hamiltonian. The spectral properties of H can be extracted from the properties of invertibility of the infinite matrix $S(E)$. Namely, at least for $E < \hbar\omega/2$ the energy E belongs to the spectrum of H if the matrix $S(E)$ is not invertible. Under so-called “rationality condition”,⁹ we can reduce the problem to invert the infinite matrix $S(E)$ to a problem of finite-dimensional algebra. According to Ref. 9, we call the field \mathbf{B} *rational* with respect to Λ if for some basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of Λ , all the numbers $\mathbf{b}(\mathbf{a}_j \times \mathbf{a}_k)$ are rational. It is clear that every \mathbf{B} obeys this condition after an appropriate infinitely small change of direction, therefore, the rationality condition imposes no essential restrictions on \mathbf{B} . If \mathbf{B} is rational with respect to Λ , then a basis \mathbf{a}_j of Λ can be chosen in such a way that $\eta \equiv \mathbf{b}(\mathbf{a}_1 \times \mathbf{a}_2) > 0$ and $\mathbf{b}(\mathbf{a}_2 \times \mathbf{a}_3) = \mathbf{b}(\mathbf{a}_1 \times \mathbf{a}_3) = 0$. Denote $\eta = N/M$, where N and M are coprime positive integers; in our approach the crucial role is played by the following $(MK) \times (MK)$ matrix \tilde{S} , where K is the number of nodes in K :

$$\begin{aligned} \tilde{S}_{q, q'}(\mathbf{p}, E) &= \exp[-\pi i m' \mathbf{b}(\boldsymbol{\kappa}' \times \mathbf{a}_2)] \\ &\times \sum_{\lambda_1, \lambda_2, \lambda_3 = -\infty}^{\infty} S(\lambda_1 \mathbf{a}_1 + (\lambda_2 M + m) \mathbf{a}_2 + \boldsymbol{\kappa}, m' \mathbf{a}_2 + \boldsymbol{\kappa}', \lambda_3 \mathbf{a}_3; E) \\ &\times \exp[\pi i (\lambda_1 \mathbf{a}_1 + (\lambda_2 M + m) \mathbf{a}_2) (\mathbf{b} \times \boldsymbol{\kappa} - \eta \lambda_1 (M \lambda_2 + m) - 2\boldsymbol{\lambda} \cdot \mathbf{p})]. \end{aligned} \quad (11)$$

Here q denotes the pair $(m, \boldsymbol{\kappa})$ with $\boldsymbol{\kappa} \in K$, $m = 0, \dots, M-1$ and \mathbf{p} is the magnetic quasi-momentum. The magnetic Brillouin zone is defined by the inequalities $0 \leq p_1 \leq M^{-1}$, $0 \leq p_2 \leq 1$, $0 \leq p_3 \leq 1$ and, in this zone, the dispersion relation for H reads

$$\det \tilde{S}(\mathbf{p}, E) = 0. \quad (12)$$

For a fixed \mathbf{p} , Eq. (12) has infinitely many solutions $E_s(\mathbf{p})$, $s = 0, 1, \dots$; each $E_s(\mathbf{p})$ is an M -fold degenerate eigenvalue of H . Dispersion laws $E = E_s(\mathbf{p})$ are continuous functions of \mathbf{p} ; the set of all values of $E_s(\mathbf{p})$ is an interval J_s . In a natural way, the intervals J_s form clusters called *magnetic bands* or *Landau bands*, each magnetic band contain KM adjacent intervals J_s (*subbands*). For the Fermi energy E_F , the equation

$$E_s(\mathbf{p}) = E_F \quad (13)$$

determines a periodic surface in the quasi-momentum space (the *Fermi surface*).

3. Results of Numerical Analysis

Using Eqs. (11)–(13) we analyze numerically the shape of the Fermi surfaces in a crystal with the simple-cubic lattice for various directions of the field \mathbf{B} . The

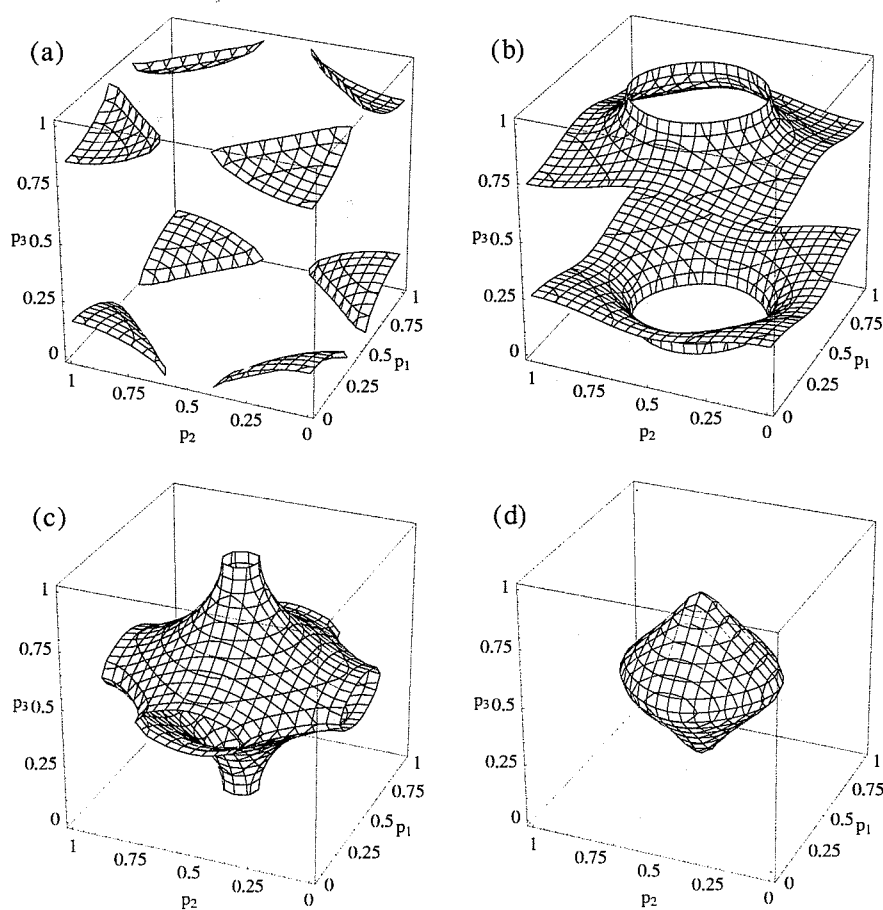


Fig. 1. The Fermi surfaces for 3D crystals with simple-cubic lattice at $\eta = 1$. The field \mathbf{B} is parallel to \mathbf{a}_3 . (a) $E_F = -1.13 \epsilon_0$; (b) $E_F = -1.06 \epsilon_0$; (c) $E_F = -0.87 \epsilon_0$; and (d) $E_F = -0.79 \epsilon_0$.

lattice constant $a = 7.5$ nm is chosen relevant to the geometric parameters for the 3D regimented quantum dot superlattice considered recently in Ref. 19. As to the scattering length, we put $\rho \sim 1$ nm, this corresponds to the binding energy $E \sim 30$ meV.

Let the magnetic field \mathbf{B} directed along the edge \mathbf{a}_3 of the cubic elementary cell and $\eta = 1$; this value of η corresponds to the field strength ~ 70 T (note in this connection that it was reported on the possibility to achieve the magnetic field strength 28 MG²⁰). In the considered case, the lowest magnetic band of the spectrum has the form $[-1.21\varepsilon_0; -0.68\varepsilon_0]$, where $\varepsilon_0 = \hbar\omega/2$. The Fermi surfaces for various energy values from this band are depicted in Fig. 1. The warped ellipsoids in panels (a) and (d) are the electron and hole surfaces, respectively; in this case *there exist only closed trajectories of the charged particle in the p-space*. Other topologies of the Fermi surface are shown in panels (b) and (c); according to the definition from Ref. 2 that these surfaces have the topology of ranges 2 and 3, respectively.

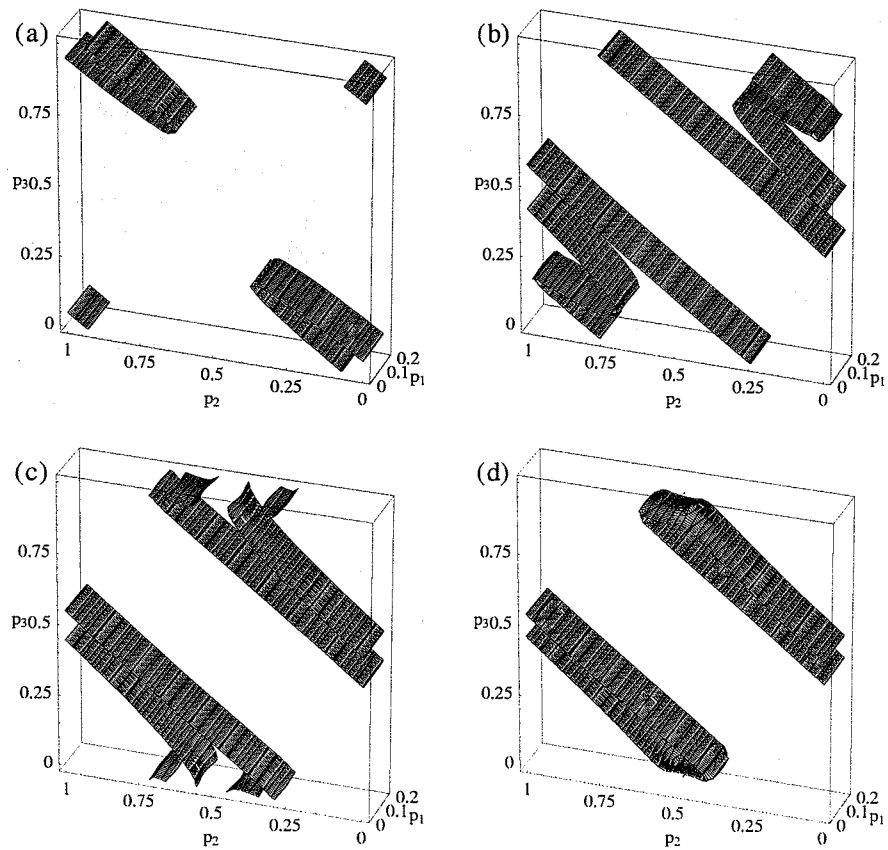


Fig. 2. The Fermi surfaces for 3D crystals with simple-cubic lattice at $\eta = 1$. Field \mathbf{B} is parallel to the plane $(y0z)$ and forms the angle $\theta = \text{atan}(3/4)$ with \mathbf{a}_3 . The Fermi energy lies in the first subband: (a) $E_F = -1.09\varepsilon_0$; (b) $E_F = -1.03\varepsilon_0$; (c) $E_F = -1.01\varepsilon_0$; and (d) $E_F = -0.99\varepsilon_0$.

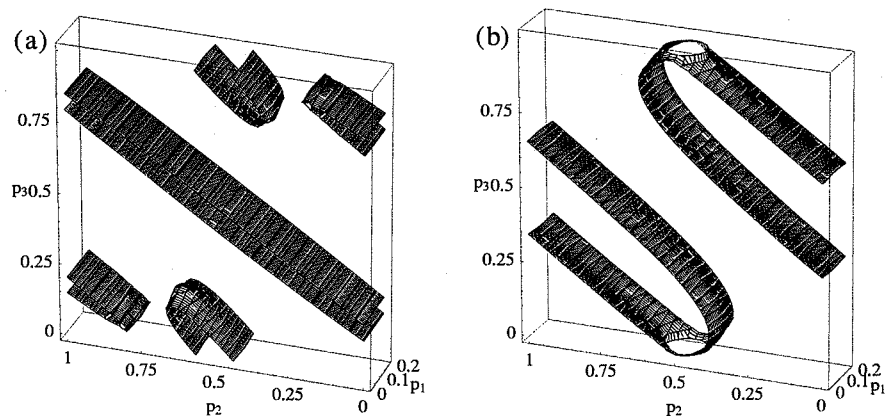


Fig. 3. The Fermi surfaces for geometry as at Fig. 2. The Fermi energy lies (a) in the second subband $E_F = -0.96 \epsilon_0$ and (b) in the fourth subband $E_F = -0.83 \epsilon_0$.

Surprisingly, an inclination of \mathbf{B} to the edge of the cubic cell causes a profound reconstruction of the Fermi surfaces. As an example we consider $\mathbf{B} = B(0, 3/5, 4/5)$. In the new basis $\mathbf{a}'_1 = \mathbf{a}_1$, $\mathbf{a}'_2 = \mathbf{a}_2 + \mathbf{a}_3$, $\mathbf{a}'_3 = 3\mathbf{a}_2 + 4\mathbf{a}_3$, we have $\mathbf{a}'_3 \parallel \mathbf{B}$ and $\eta = 1/5$. Therefore, the magnetic Brillouin zone is defined by the inequalities $0 \leq p_1 \leq 1/5$, $0 \leq p_2, p_3 \leq 1$, and the lowest magnetic band splits into five subbands. Figure 2 shows the variation of the Fermi surface as the Fermi energy E_F varies in the first subband $[-1.11 \epsilon_0; -0.98 \epsilon_0]$. The electron and hole Fermi surfaces have the shapes of warped cylinders (panels (a) and (d), respectively) or highly-twisted sheets (panels (b) and (c)). It is particularly remarkable that in this case the surfaces are open in the p_1 -direction. In going from the first subband of the lowest magnetic band to the higher subbands, the shape of the Fermi surface changes; examples of this change are shown on Fig. 3, where the Fermi energy E_F lies in the second and fourth subbands, respectively.

In the examples above, the field \mathbf{B} is parallel to a face of the cubic cell. We have built the Fermi surface for the field of the form $\mathbf{B} = B(12/25, 9/25, 4/25)$, where $\eta = 1/25$ but by the technical reasons do not give the corresponding figure here. In this case, the Fermi surface is divided into great numbers of connected pieces having the shape of winding sheets.

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