Coulomb Breakup Problem

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We formulate scattering theory in the framework of a surface-integral approach utilizing analytically known asymptotic forms of the three-body wave functions. This formulation is valid for both short-range and Coulombic potentials. The post and prior forms of the breakup amplitude are derived without any reference to renormalization procedures.

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Scattering in a few-body system is one of the central subjects of quantum mechanics. However, conventional scattering theory is formally valid only when the particles interact via short-range potentials. For charged particles with the long-range Coulombic interactions the theory requires modification. In the time-dependent formulation, formal scattering theory is generalized to include Coulombic potentials by choosing appropriately modified time evolution operators [1]. This is equivalent to various forms of screening and renormalization [2–4] in the time-independent formulation. The renormalization method leads to the correct cross sections for the two-body problem; however, the results from this procedure cannot be regarded as completely satisfactory. For instance, different ways of screening lead to different asymptotic forms for the scattering wave function. Generally, these asymptotic forms differ from the exact one obtained from the solution of the Schrödinger equation (SE). Moreover, they give rise to a scattering amplitude that does not exist on the energy shell due to divergent complex factors [4,5]. These factors must be removed (renormalized) before approaching the on-shell point. But the renormalization factors depend on the way the limits are taken when the on-shell point is approached. In other words, depending on the way the limits are taken different factors need to be removed. Thus, the *ad hoc* renormalization procedure is based on prior knowledge of the exact answer to compare with and has no *ab initio* theoretical justification. Recently we have demonstrated that there was a general approach to the two-body collision problem [6] that did not lead to the aforementioned formal difficulties and did not require renormalization.

The situation in a few-body system is even more complicated. Rigorous scattering theory for a system of three particles valid for short-range potentials was given by Faddeev [7]. A renormalization method was implemented successfully for the three-body problem when only two particles are charged [8]. Though Dollard's time-dependent approach [1] is believed to be formally valid for arbitrary multichannel collisions, it has not developed into a practical method for calculations. At the same time, no practical renormalization method exists that is valid for a system of three charged particles above the breakup threshold either. The problem is that above the threshold the Coulomb three-body system possesses essentially different types of singularities and the two-particle renormalization procedures are not sufficient to guarantee compactness of the Faddeev equations [3,9]. Thus there is no theoretical proof or practical evidence that a renormalization approach can be applied to the system of three charged particles.

Another issue hindering a complete formal understanding of the breakup process is how to extract the scattering information from the wave function when the latter is available. To be more specific, for three charged particles the theory fails to provide a formal post form definition for the scattering amplitude in terms of the total wave function with outgoing scattered waves. Therefore, the Coulomb interaction is screened and the formula for the short-range case is used.

Thus we have a situation when we cannot use the theory unless we screen the Coulomb interaction. And when we do, we end up with quantities which diverge as screening is removed. This leaves no choice but to invoke renormalization to fix unphysical results. Therefore, a new approach to Coulomb few-body problems that does not need renormalization is required. The variational approach [10] is a step forward in this direction. However, this approach leads to the transition amplitudes which also contain oscillatory divergences but for different reasons. It was suggested that these divergences can be made to vanish using ''radius averaging'' procedure [10]. The method has been extended to charged particles in Ref. [11].

There are sophisticated numerical approaches to solving three-body scattering problems in nuclear physics with two charged particles. Some [12–14] are based on the Faddeev [7] and Alt-Grassberger-Sandhas [15] equations. Others tackle the same problem through direct numerical solution of the relevant SE for the scattering wave function [16,17] or using variational techniques [18]. The Coulomb interaction between the two protons has been fully included in the calculation of proton-deuteron breakup for the first time in Ref. [13]. However, due to formal problems mentioned earlier no such strict approach for breakup processes

in nuclear three-body systems, when all particles are charged, has been developed. For this reason calculations of $(p, 2p)$ and similar nuclear breakup reactions with three charged particles in the final state have been limited to high energies where distorted-wave Born-type approaches are applicable.

In atomic physics, despite the above-mentioned formal difficulties, surprising progress has been achieved in describing $(e, 2e)$ processes via the exterior complex scaling (ECS) [19–21] and the convergent close coupling (CCC) [22,23] methods. The success of the ECS approach to Coulomb breakup problems, in particular, caused us to reexamine the underlying formal theory [24]. The amplitude is calculated from Peterkop's trial integral [25] that has phase ambiguity and divergence problems. In the CCC method one of the electrons is treated using a square-integrable representation, and the breakup amplitude can also be related to a particular form of Peterkop's trial integral. Despite the success of the computational methods, in describing the measured cross sections, the traditional formal theory of scattering is unable to show how to calculate the breakup amplitude unambiguously and in a divergence-free manner. The conventional formal theory is also not capable of explaining the origin of the trial integral which is the cornerstone of the aforementioned methods.

In this Letter we present a surface-integral approach to formulating scattering theory. We use the recently derived analytic results for total scattering wave functions in asymptotic domains [9,26–28] to develop a well-defined prior and post forms of the breakup amplitude valid for short-range and Coulombic potentials. These new definitions do not require screening and renormalization or any regularization as they are exact and divergence-free.

Let us consider a system of three particles of mass m_α and charge z_α, $\alpha = 1, 2, 3$. We use Jacobi coordinates where $\boldsymbol{r}_\alpha$ and $\boldsymbol{k}_\alpha$ are, respectively, the relative coordinate and momentum between particles β and γ. The coordinate of particle α relative to the center of mass of the pair (β, γ) is $\boldsymbol{\rho}_\alpha$, with $\boldsymbol{q}_\alpha$ being the canonically conjugate relative momentum. The corresponding reduced masses are denoted by $\mu_\alpha = m_\beta m_\gamma/(m_\beta + m_\gamma)$ and $M_\alpha = m_\alpha(m_\beta + m_\gamma)/(m_\alpha + m_\beta + m_\gamma)$. We also introduce a hyperradius in the six-dimensional configurations space $R = (\mu_\alpha/\mu r_\alpha^2 + M_\alpha/\mu\rho_\alpha^2)^{1/2}$, where μ is an arbitrary mass constant introduced for convenience (the final results do not depend on this complementary constant), and a five-dimensional hyperangle $\omega = (\hat{\boldsymbol{r}}_\alpha, \hat{\boldsymbol{\rho}}_\alpha, \varphi_\alpha)$ with $\varphi_\alpha = \arctan[(\mu_\alpha/M_\alpha)^{1/2} r_\alpha/\rho_\alpha]$, $0 \le \varphi_\alpha \le \pi/2$. Indeces α, β, γ are cyclic. We use n to specify a full set of quantum numbers of a bound state.

Consider now scattering of particle α with incident momentum $\boldsymbol{q}_{\alpha n}$ off a bound pair (β, γ) in initial state $\phi_{\alpha n}$ of energy $E_{\alpha n}$. Assume that the energy of the projectile $q_{\alpha n}^2/2M_\alpha$ is sufficient to break up the target. The total wave function describing this process satisfies the SE

$$(E - H)\Psi_{\alpha n}^{+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0, \tag{1}$$

with outgoing-spherical wave boundary conditions. Here $H = H_0 + V$, $H_0 = -\Delta_{\boldsymbol{r}_\alpha}/2\mu_\alpha - \Delta_{\boldsymbol{\rho}_\alpha}/2M_\alpha$, $V = v + V_\alpha + V_\beta + V_\gamma$ is the full interaction, v is a three-body interaction and V_α is a Coulombic interaction between particles β and γ, $E = E_{\alpha n} + q_{\alpha n}^2/2M_\alpha = k_\alpha^2/2\mu_\alpha + q_\alpha^2/2M_\alpha$ is the total energy of the system. There is another process which may take place within the same system at the same energy E called $3 \to 3$ scattering. The wave function Ψ_0^- describing this process is also an eigenstate of the same Hamiltonian H; however, we impose incoming-wave boundary conditions on it. It develops to the final state where all three particles are in the continuum.

In scattering theory we deal with functions which are not square-integrable (L^2). While this fact is not a problem on its own, nevertheless, non-L^2 functions do make certain integrals emerging in the theory divergent. In case of integrals containing the interaction potential a standard procedure, which ensures their existence, is limiting the range of the potential. This irreversibly distorts the nature of the problem. Instead, we first formulate the scattering problem in a finite region of coordinate space and then extend it to the full space. To this end we introduce a partial inner product of two arbitrary functions Ψ_i and Ψ_f in the space of functions describing various states and arrangements in a three-body system according to $\langle\Psi_f|\Psi_i\rangle_{R_0} = \int_{R\le R_0} d\boldsymbol{r}_\alpha d\boldsymbol{\rho}_\alpha \Psi_f^* \Psi_i$, where the integration is limited to the volume of a six-dimensional hyperball of radius R_0.

We want to use $\Psi_{\alpha n}^+$ and Ψ_0^- as starting points to derive prior and post forms of the breakup amplitude. If we split $\Psi_{\alpha n}^+$ into the initial-channel wave $\Phi_{\alpha n}^+$ and scattered wave $\Psi_{\alpha n}^{\mathrm{sc}+}$ then Eq. (1) transforms to

$$(E - H)\Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = (H - E)\Phi_{\alpha n}^{+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha). \tag{2}$$

We multiply Eq. (2) by Ψ_0^{-*} from the left and integrate the result over a volume of a hyperball of radius R_0:

$$\langle\Psi_0^-|(E - H)\Psi_{\alpha n}^{\mathrm{sc}+}\rangle_{R_0} = \langle\Psi_0^-|(H - E)\Phi_{\alpha n}^{+}\rangle_{R_0}. \tag{3}$$

We assume V to be real. Then we have $\langle(E - H)\Psi_0^-|\Psi_{\alpha n}^{\mathrm{sc}+}\rangle_{R_0} = 0$, which is true for any R_0 simply due to $(E - H)\Psi_0^- = 0$. Now we subtract this from Eq. (3). Despite the fact that both Ψ_0^- and $\Psi_{\alpha n}^{\mathrm{sc}+}$ are non-L^2 functions, terms of the form $\langle\Psi_0^-|(E - V)\Psi_{\alpha n}^{\mathrm{sc}+}\rangle_{R_0}$ are finite due to the limited space. Therefore, canceling them we get

$$-\langle\Psi_0^-|H_0\Psi_{\alpha n}^{\mathrm{sc}+}\rangle_{R_0} + \langle H_0\Psi_0^-|\Psi_{\alpha n}^{\mathrm{sc}+}\rangle_{R_0} = \langle\Psi_0^-|(H - E)\Phi_{\alpha n}^{+}\rangle_{R_0}. \tag{4}$$

Now we investigate the limit of this equation as $R_0 \to \infty$. What does $\lim_{R_0\to\infty}\langle\Psi_0^-|(H - E)\Phi_{\alpha n}^{+}\rangle_{R_0}$ represent? In order to see this we evaluate the limit of the left-hand side (LHS) of Eq. (4).

An essential feature of the term on the LHS of Eq. (4) is that it is easily transformed into an integral over the hypersurface of radius R_0 so that the result depends only on the behavior of the wave functions on this surface. Therefore,

the knowledge of the wave functions anywhere inside the surface is not required. Then it can be evaluated using the asymptotic forms of the wave functions. We consider two distinct asymptotic domains. We call Ω_0 the domain whenever all interparticle distances are large, i.e., $r_\alpha \to \infty$, $\rho_\alpha \to \infty$, so that r_α/ρ_α is nonzero. In addition, we call Ω_α the asymptotic regime where $\rho_\alpha \to \infty$; however, r_α satisfies the constraint $r_\alpha/\rho_\alpha \to 0$. Parameter R_0 can go to infinity with the system being in Ω_0 or Ω_α. If $R_0 \to \infty$ in Ω_0 then for the limit of the LHS of Eq. (4) we have

$$\frac{\mu^2}{2(\mu_\alpha M_\alpha)^{3/2}} \lim_{R_0\to\infty} R_0^5 \int d\hat{\boldsymbol{r}}_\alpha d\hat{\boldsymbol{\rho}}_\alpha \int_0^{\pi/2} d\varphi_\alpha \sin^2\varphi_\alpha \cos^2\varphi_\alpha \left[\Psi_0^{-*} \frac{\partial}{\partial R} \Psi_{\alpha n}^{\mathrm{sc}+} - \Psi_{\alpha n}^{\mathrm{sc}+} \frac{\partial}{\partial R} \Psi_0^{-*} \right]_{R=R_0}. \tag{5}$$

Here we first transformed H_0 into (R, ω) variables and then used Green's theorem to transform the volume integral into the surface one. The wave function Φ_0^- (a part of Ψ_0^-) in Ω_0 was given by Redmond [29]. Using this and the asymptotic forms for $\Psi_{\alpha n}^{\mathrm{sc}+}$ [9,27] and $\Psi_0^{\mathrm{sc}-}$ [28], and performing differentiation we get for Eq. (5), to the leading order in R_0,

$$\begin{aligned}
&\frac{\kappa^{3/2}}{k_\alpha q_\alpha} \frac{(\mu_\alpha M_\alpha)^{1/2}}{\sqrt{8\pi}\mu} \lim_{R_0\to\infty} R_0^{1/2} e^{i\kappa R_0} \int_0^{\pi/2} d\varphi_\alpha \sin\varphi_\alpha \cos\varphi_\alpha e^{-i\lambda_0 \ln(2\kappa R_0) - i\sigma_0} \left(\kappa + \sqrt{\frac{\mu}{\mu_\alpha}} k_\alpha \sin\varphi_\alpha + \sqrt{\frac{\mu}{M_\alpha}} q_\alpha \cos\varphi_\alpha \right) \\
&\quad \times \exp\left[-i\sqrt{\frac{\mu}{\mu_\alpha}} k_\alpha R_0 \sin\varphi_\alpha - i\sqrt{\frac{\mu}{M_\alpha}} q_\alpha R_0 \cos\varphi_\alpha \right] \prod_{\nu=1,2,3} \exp\left[\frac{i\eta_\nu}{k_\nu} \ln\left(2\sqrt{\frac{\mu}{\mu_\nu}} R_0 \sin\phi_\nu k_\nu \right) \right] \\
&\quad \times T\left(\sqrt{\frac{\mu_\alpha}{\mu}} \kappa \sin\varphi_\alpha \hat{\boldsymbol{k}}_\alpha, \sqrt{\frac{M_\alpha}{\mu}} \kappa \cos\varphi_\alpha \hat{\boldsymbol{q}}_\alpha \right).
\end{aligned} \tag{6}$$

Here σ_0 and λ_0 are slowly-varying functions of φ_α that do not depend on R_0, and T is the amplitude of the scattered wave $\Psi_{\alpha n}^{\mathrm{sc}+}$ in Ω_0 [27]; i.e., it is the breakup amplitude. This is an extremely oscillatory integral as $R_0 \to \infty$ and therefore, only points of stationary phase in φ_α, if there are any, contribute to the integral. There is such a point at $\sin\varphi_\alpha = \sqrt{\mu/\mu_\alpha} k_\alpha/\kappa$ where $\cos\varphi_\alpha = \sqrt{\mu/M_\alpha} q_\alpha/\kappa$. Calculating the remaining integral by means of the stationary-phase method we find that Eq. (6) reduces to $T(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha)$ indicating that the limit of the LHS of Eq. (4) is in fact equal to the breakup amplitude. Therefore, the limit of Eq. (4) is written as

$$T(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = \lim_{R_0\to\infty} \langle \Psi_0^- | (H - E) \Phi_{\alpha n}^+ \rangle_{R_0}. \tag{7}$$

In other words, if scattering takes place into Ω_0 domain then $\lim_{R_0\to\infty} \langle \Psi_0^- | (H - E) \Phi_{\alpha n}^+ \rangle_{R_0}$ does exist, and is the breakup amplitude regardless of the nature of the interaction potentials.

If the products of scattering turn out to be in Ω_α or Ω_β domains then we have to differentiate whether all three particles are in the continuum or just one. If all three are in the continuum then in a similar way we used for Ω_0 we again arrive at Eq. (7). The only difference is that in these domains we use for Φ_0^- the form given by Alt and Mukhamedzhanov [26]. Thus, Eq. (7) defines the breakup amplitude in all asymptotic domains corresponding to breakup.

We can also start from Ψ_0^-. If we separate Ψ_0^- into Coulomb-distorted three-body plane wave Φ_0^- and scattered wave $\Psi_0^{\mathrm{sc}-}$ then the SE for Ψ_0^- is written as

$$(E - H) \Psi_0^{\mathrm{sc}-}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = (H - E) \Phi_0^-(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha). \tag{8}$$

Let us take the complex conjugate of Eq. (8) and multiply it by $\Psi_{\alpha n}^+$ from the right. Then integrating the result over the volume of a hyperball of radius R_0 we get

$$\langle (E - H) \Psi_0^{\mathrm{sc}-} | \Psi_{\alpha n}^+ \rangle_{R_0} = \langle (H - E) \Phi_0^- | \Psi_{\alpha n}^+ \rangle_{R_0}. \tag{9}$$

From Eq. (1) we have $\langle \Psi_0^{\mathrm{sc}-} | (E - H) \Psi_{\alpha n}^+ \rangle_{R_0} = 0$. Subtracting this from Eq. (9) we obtain

$$\begin{aligned}
&- \langle H_0 \Psi_0^{\mathrm{sc}-} | \Psi_{\alpha n}^+ \rangle_{R_0} \\
&\quad + \langle \Psi_0^{\mathrm{sc}-} | H_0 \Psi_{\alpha n}^+ \rangle_{R_0} = \langle (H - E) \Phi_0^- | \Psi_{\alpha n}^+ \rangle_{R_0}.
\end{aligned} \tag{10}$$

We again investigate the limit of this equation as $R_0 \to \infty$. However, this time we have the situation of three free particles in the initial state. In the final state we may have three free particles or two of the particles may form a bound state. These events correspond to cases when $R_0 \to \infty$ in Ω_0 or Ω_α, respectively. Let us consider the latter case, corresponding to recombination. In this case the limit of LHS of Eq. (10) is written as

$$\begin{aligned}
&\frac{1}{2M_\alpha} \lim_{R_0\to\infty} R_0^2 \int d\boldsymbol{r}_\alpha d\hat{\boldsymbol{\rho}}_\alpha \left[\Psi_{\alpha n}^+ \frac{\partial}{\partial \rho_\alpha} \Psi_0^{\mathrm{sc}-*} \right. \\
&\qquad \left. - \Psi_0^{\mathrm{sc}-*} \frac{\partial}{\partial \rho_\alpha} \Psi_{\alpha n}^+ \right]_{\rho_\alpha = R_0}.
\end{aligned} \tag{11}$$

An essential difference from Eq. (5) here is that only one of the three-dimensional volume integrals is transformed into the surface integral. The remaining volume integral is limited due to presence of a bound state in channel α. In order to calculate Eq. (11) we need the asymptotic forms of $\Psi_0^{\mathrm{sc}-}$ and $\Psi_{\alpha n}^+$ in Ω_α. They have been given in Refs. [9,27,28]. Using these and evaluating the integral by the stationary-phase method we find that Eq. (11) reduces to $F^*(\boldsymbol{q}_{\alpha n}; \boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha)$, where F is the amplitude for recombination of three free particles into two-fragment channel state αn. According to the reciprocity principle

$F^* = T$. Therefore, the limit of Eq. (10) is in fact written as

$$T(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = \lim_{R_0 \to \infty} \langle (H - E)\Phi_0^- | \Psi_{\alpha n}^+ \rangle_{R_0}. \quad (12)$$

This means that $\lim_{R_0\to\infty}\langle (H - E)\Phi_0^- | \Psi_{\alpha n}^+ \rangle_{R_0}$ also exists and also represents the breakup amplitude.

Incidentally, the same analysis can be performed on the right-hand side of Eqs. (7) and (12) to yield $T(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha)$. Thus, the general volume-integral prior and post forms of the breakup amplitude are written as

$$T^{\text{prior}}(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = \langle \Psi_0^- | (H - E)\Phi_{\alpha n}^+ \rangle, \quad (13)$$

$$T^{\text{post}}(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = \langle (H - E)\Phi_0^- | \Psi_{\alpha n}^+ \rangle, \quad (14)$$

which are valid for both short-range and Coulombic potentials. These new definitions are consistent with the well-known ones for short-range interactions. To see this we note that when the interactions are short ranged we have $\Phi_{\alpha n}^+(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \to e^{i\boldsymbol{q}_{\alpha n}\boldsymbol{\rho}_\alpha}\phi_{\alpha n}(\boldsymbol{r}_\alpha)$. This leads to

$$(H - E)\Phi_{\alpha n}^+(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = (V - V_\alpha)e^{i\boldsymbol{q}_{\alpha n}\boldsymbol{\rho}_\alpha}\phi_{\alpha n}(\boldsymbol{r}_\alpha). \quad (15)$$

At the same time if we have three particles in the final channel then $\Phi_0^-(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \to e^{i\boldsymbol{k}_\alpha\boldsymbol{r}_\alpha + i\boldsymbol{q}_\alpha\boldsymbol{\rho}_\alpha}$. Then we have

$$(H - E)\Phi_0^-(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = Ve^{i\boldsymbol{k}_\alpha\boldsymbol{r}_\alpha + i\boldsymbol{q}_\alpha\boldsymbol{\rho}_\alpha}. \quad (16)$$

Therefore, the general forms of the amplitudes (13) and (14) reduce to the standard definitions for short-range interactions

$$T^{\text{prior}}(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = \langle \Psi_0^- | V - V_\alpha | \phi_{\alpha n}, \boldsymbol{q}_{\alpha n} \rangle, \quad (17)$$

$$T^{\text{post}}(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = \langle \boldsymbol{q}_\alpha, \boldsymbol{k}_\alpha | V | \Psi_{\alpha n}^+ \rangle. \quad (18)$$

Equation (14) in part explains the success of the integral formula used in atomic breakup problems. As mentioned earlier, the ECS approach [20] is based on Peterkop's integral, $\langle (H - E)\Phi_{z_1,z_2}^- | \Psi_{\alpha n}^+ \rangle$, where Φ_{z_1,z_2}^- is a trial function taken as a product of two Coulomb waves of effective charges z_1 and z_2 which should satisfy a certain condition [25]. As we can see from Eq. (14), the Peterkop integral is simply an approximation to the exact breakup amplitude in its post form, where the exact three-body state Φ_0^- is replaced by the trial function. The breakup amplitude in the ECS approach is calculated by taking $z_1 = z_2 = 1$. Such a choice of the effective charges does not satisfy the aforementioned condition. However, remarkably, it turns out that with any choice of the effective charges the difference between the breakup amplitude and Peterkop's integral reduces to a phase factor which does not affect the cross sections [24]. The CCC method [23] in effect uses the Peterkop trial integral, with the L^2 expansion of the target space requiring $z_1 = 0$ and $z_2 = 1$. We believe that the new forms for the breakup amplitude given in this Letter will be just as successful in solving nuclear breakup problems with charged particles.

Summarizing, we have derived for the first time post and prior forms of the breakup amplitude for a three-body system that are valid for both short-range and Coulombic potentials. This was made possible by the recently obtained analytic forms of the asymptotic wave functions combined with a surface integral approach to the scattering theory. No requirement for screening or renormalization has been necessary. Full details will be given elsewhere.

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