

Strength of reduced two-body spin-orbit interaction from a chiral three-nucleon force

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The contribution of the chiral three-nucleon force to the strength of effective spin-orbit coupling is estimated. We construct a reduced two-body interaction by folding single-nucleon degrees of freedom of the three-nucleon force in nuclear matter. The spin-orbit strength is evaluated by the Scheerbaum factor obtained by a G -matrix calculation in nuclear matter with the two-nucleon interaction plus the reduced two-nucleon interaction. The inability of modern realistic two-nucleon interactions to account for the empirical spin-orbit strength is overcome. We found that spin-orbit coupling is weaker in a neutron-rich environment. Because the spin-orbit component of the three-nucleon force is determined by low-energy constants fixed in the two-nucleon sector, the present estimation has a small uncertainty.

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The spin-orbit field in atomic nuclei is essential for reproducing the well-established single-particle shell structure. However, the empirical strength of the spin-orbit potential has not been fully explained in terms of a realistic nucleon-nucleon force. Fujita and Miyazawa [1] considered the possible effect of intermediate isobar Δ excitation on the nuclear spin-orbit field, which followed the construction of the two-pion-exchange three-nucleon force (3NF). This problem was reinvestigated in the early 1980s [2,3] to search for the additional spin-orbit strength. The Illinois group [4,5] later showed that the 3NF makes a substantial contribution to spin-orbit splitting in ^{15}N .

Kaiser and collaborators [6–8] investigated nuclear spin-orbit coupling in the framework of chiral perturbation theory. The large contributions of iterated one-pion exchange and the 3NF almost cancel each other [6,7] and the short-range spin-orbit strength in the form of effective four-nucleon contact coupling deduced from realistic nucleon-nucleon interactions accounts well [8] for the empirical spin-orbit strength. However, because the contact interaction in the chiral perturbation needs to be regulated when applying it in low-energy nuclear structure calculations and their arguments for various contributions do not seem to be fully unified, it is worthwhile to analyze the effective spin-orbit coupling strength by applying the established microscopic theory, namely lowest-order Brueckner theory (LOBT), to two- and three-nucleon interactions in chiral effective field theory (Ch-EFT).

The Thomas form of the average single-particle spin-orbit potential has been used to describe nucleon spin-orbit coupling:

$$U_{\ell s}^0 \frac{1}{r} \frac{d\rho(r)}{dr} \boldsymbol{\ell} \cdot \boldsymbol{\sigma}, \quad (1)$$

where the radial function $\rho(r)$ is the total nucleon density distribution. Scheerbaum [9] derived the relation between the strength $U_{\ell s}^0$ and the two-body effective spin-orbit interaction. We define the constant $B_S(\bar{q})$ for the spin-triplet odd-parity component of the effective two-body spin-orbit interaction

$v_{\ell s}^{3O}(r)$ as

$$B_S(\bar{q}) = -\frac{2\pi}{\bar{q}} \int_0^\infty dr r^3 j_1(\bar{q}r) v_{\ell s}^{3O}(r), \quad (2)$$

where j_1 is the spherical Bessel function. The single-particle spin-orbit potential for spin-saturated nuclei can then be written as

$$U_{\ell s, \tau}(r) = \frac{1}{2} B_S(\bar{q}) \frac{1}{r} \frac{d\{\rho(r) + \rho_\tau(r)\}}{dr} \boldsymbol{\ell} \cdot \boldsymbol{\sigma}, \quad (3)$$

where τ specifies a proton or neutron. We refer to $B_S(\bar{q})$ as the Scheerbaum factor; it differs from the constant used in Ref. [9] by a factor of $-\frac{2\pi}{3}$. Scheerbaum prescribed $\bar{q} \approx 0.7 \text{ fm}^{-1}$ based on the wavelength of the density distribution. We employ this prescription. Assuming the naive relation $\rho_p(r) = \rho_n(r) = \frac{1}{2}\rho(r)$, we recover the Thomas form, Eq. (1), with $U_{\ell s}^0 = \frac{3}{4} B_S(\bar{q})$. It has been customary to use the following δ -type two-body spin-orbit interaction,

$$i W(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot [\nabla_r \times \delta(\mathbf{r}) \nabla_r], \quad (4)$$

in nuclear Hartree-Fock calculations using δ -type Skyrme interactions [10,11] and even with finite-range effective forces (e.g., the Gogny force [12]). This two-body force provides the following single-particle spin-orbit potential:

$$\frac{1}{2} W \frac{1}{r} \frac{d\{\rho(r) + \rho_\tau(r)\}}{dr} \boldsymbol{\ell} \cdot \boldsymbol{\sigma}. \quad (5)$$

Therefore, the strength W may be equated with the Scheerbaum factor $B_S(\bar{q})$. The empirical value of W is about 120 MeV fm^5 in various nuclear Hartree-Fock calculations. As we show below, modern nucleon-nucleon interactions underestimate the spin-orbit strength by about 25%.

By applying Scheerbaum's formulation to the momentum-space G -matrix calculation in nuclear matter with the Fermi momentum k_F , we obtain the corresponding spin-orbit strength as follows [13]:

$$\begin{aligned} B_S(\bar{q}) = & \frac{1}{k_F^3} \sum_{JT} (2J+1)(2T+1) \int_0^{q_{\max}} dq \\ & \times W(\bar{q}, q) \{ (J+2) G_{1J+1, 1J+1}^{JT}(q) + G_{1J, 1J}^{JT}(q) \\ & - (J-1) G_{1J-1, 1J-1}^{JT}(q) \}. \end{aligned} \quad (6)$$

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TABLE I. $B_S(\bar{q})$ in units of MeV fm^5 given by Eq. (6) with $\bar{q} = 0.7 \text{ fm}^{-1}$ for modern nucleon-nucleon interaction: AV18 [20], NSC97 [21], CD-Bonn [23], and Jülich N^3LO [22]. The last entry is the result obtained when the reduced two-body interaction from the Ch-EFT 3NF is included.

$k_F = 1.35 \text{ fm}^{-1}$	AV18	NSC97	CD-B	N^3LO	$\text{N}^3\text{LO} + 3\text{NF}$
$B_S(T=0)$	2.0	1.9	3.1	2.5	7.0
$B_S(T=1)$	86.4	86.7	90.2	84.6	116.2
$B_S(\bar{q})$	88.4	88.6	93.3	87.1	123.2
$k_F = 1.07 \text{ fm}^{-1}$	AV18	NSC97	CD-B	N^3LO	$\text{N}^3\text{LO} + 3\text{NF}$
$B_S(T=0)$	1.4	1.3	2.3	1.6	4.1
$B_S(T=1)$	88.1	88.7	92.2	86.5	106.7
$B_S(\bar{q})$	89.5	90.0	94.5	88.1	110.8

Here, $q_{\text{max}} = \frac{1}{2}(k_F + \bar{q})$ and the weight factor $W(\bar{q}, q)$ is given by

$$W(\bar{q}, q) = \begin{cases} \theta(k_F - \bar{q}) & \text{for } 0 \leq q \leq \frac{|k_F - \bar{q}|}{2} \\ \frac{k_F^2 - (\bar{q} - 2q)^2}{8\bar{q}q} & \text{for } \frac{|k_F - \bar{q}|}{2} \leq q \leq \frac{k_F + \bar{q}}{2}, \end{cases} \quad (7)$$

where $\theta(k_F - \bar{q})$ is a step function. In Eq. (6), $G_{1\ell', 1\ell}^{JT}$ indicates the momentum-space diagonal G -matrix element in the spin-triplet channel with a total isospin T , total spin J , and orbital momenta ℓ' and ℓ .

Calculating $B_S(\bar{q})$ in the lowest-order Brueckner theory with the continuous prescription for intermediate spectra, as presented explicitly in Table I, modern two-body nucleon-nucleon potentials are found to give smaller values (around 90 MeV fm^5) than the empirical one. It is well known that LOBT calculations in symmetric nuclear matter with a realistic two-nucleon force do not correctly reproduce the saturation properties. However, in most cases, calculated energies at the empirical saturation point $k_F = 1.35 \text{ fm}^{-1}$ are close to the empirical energy of about -16 MeV . This suggests that G matrices provide basic information on the effective nucleon-nucleon interaction in the nuclear medium by incorporating important short-range correlations as well as Pauli and dispersion effects.

We now consider the contribution of the 3NF. In this study, we estimate it in a two-step procedure. First, the 3NF v_{123} defined in momentum space is reduced to an effective two-nucleon interaction $v_{12(3)}$ by folding the single-nucleon degrees of freedom:

$$\begin{aligned} & \langle \mathbf{k}'_1 \sigma'_1 \tau'_1, \mathbf{k}'_2 \sigma'_2 \tau'_2 | v_{12(3)} | \mathbf{k}_1 \sigma_1 \tau_1, \mathbf{k}_2 \sigma_2 \tau_2 \rangle_A \\ &= \frac{1}{3} \sum_{\mathbf{k}_3 \sigma_3 \tau_3} \langle \mathbf{k}'_1 \sigma'_1 \tau'_1, \mathbf{k}'_2 \sigma'_2 \tau'_2, \mathbf{k}_3 \sigma_3 \tau_3 | \\ & \quad \times v_{123} | \mathbf{k}_1 \sigma_1 \tau_1, \mathbf{k}_2 \sigma_2 \tau_2, \mathbf{k}_3 \sigma_3 \tau_3 \rangle_A. \end{aligned} \quad (8)$$

Here, we assume that the two remaining nucleons are in the center-of-mass frame, namely $\mathbf{k}'_1 + \mathbf{k}'_2 = \mathbf{k}_1 + \mathbf{k}_2 = 0$. The density-dependent effective two-nucleon interaction has been commonly introduced as an effect of the 3NF [14–16]. The suffix A denotes an antisymmetrized matrix element, namely $|ab\rangle_A \equiv |ab - ba\rangle$ and $|abc\rangle_A \equiv |abc - acb + bca - bac + cab - cba\rangle$, and the factor $\frac{1}{3}$ in Eq. (8) is an additional statistical factor required to evaluate the total energy, as was

noted by Hebeler and Schwenk [17]. Previous studies have often omitted this statistical factor. If an adjustable strength is introduced, the statistical factor may be hidden in the fitting procedure. In the present case, we use the Ch-EFT 3NF and the low-energy constants except for c_D and c_E are fixed. Although there may be room to adjust c_D and c_E , these terms make rather small contributions to the energy if they lie in a reasonable range. In addition, c_D and c_E do not contribute to the reduced two-nucleon spin-orbit interaction. By comparing the nuclear matter energy calculated directly from v_{123} with that obtained by the reduced $v_{12(3)}$, the error due to this approximation was found to be less than 10%, if we calculate Born energy without including a form factor. Although it is not obvious that the statistical factor $\frac{1}{3}$ can be applied to higher order terms summed in the G -matrix evaluation, we assume that this prescription estimates the leading effect of the 3NF. More rigorous calculations of the 3NF contribution require a systematic method such as the coupled-cluster method, as the present author and Okamoto demonstrated in Ref. [18].

To explain the procedure for obtaining $v_{12(3)}$ more explicitly, we write the reduced spin-orbit component originating from the c_1 term of the Ch-EFT 3NF:

$$-\frac{c_1 g_A^2 m_\pi^2}{f_\pi^4} \sum_{1 \leq i < j \leq 3} \frac{(\boldsymbol{\sigma}_i \cdot \mathbf{q}_i)(\boldsymbol{\sigma}_j \cdot \mathbf{q}_j)}{(\mathbf{q}_i^2 + m_\pi^2)(\mathbf{q}_j^2 + m_\pi^2)} (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j), \quad (9)$$

where $g_A = 1.29$, $f_\pi = 92.4 \text{ MeV}$, m_π is the pion mass, and \mathbf{q}_i is the momentum transfer of the i th nucleon. The momentum transfer of the third nucleon k is given by $\mathbf{q}_k = -\mathbf{q}_i - \mathbf{q}_j$. The Ch-EFT 3NF has a structure similar to that of the conventional 3NF [5], which is due to P -wave scattering through isobar Δ excitation and S -wave scattering.

The folding of the 3NF by the third nucleon in a Fermi sea is performed without incorporating a three-body form factor. A form factor is later introduced on the two-body level. The folding in symmetric nuclear matter with the Fermi momentum k_F gives, besides the central and tensor components, the following spin-orbit term:

$$\begin{aligned} & \frac{c_1 g_A^2 m_\pi^2}{f_\pi^4} \frac{1}{(2\pi)^3} \int \int \int_{|\mathbf{k}_3| \leq k_F} d\mathbf{k}_3 \\ & \times \frac{i(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot [-\mathbf{k}'_1 \times \mathbf{k}_1 + (\mathbf{k}'_1 - \mathbf{k}_1) \times \mathbf{k}_3]}{[(\mathbf{k}'_1 - \mathbf{k}_3)^2 + m_\pi^2][(\mathbf{k}_1 - \mathbf{k}_3)^2 + m_\pi^2]}. \end{aligned} \quad (10)$$

When performing the folding in pure neutron matter, the restriction on the isotopic spin generates an additional factor of $\frac{1}{3}$.

The partial-wave decomposition of the above spin-orbit term becomes

$$\begin{aligned} & -\delta_{S1} \frac{c_1 g_A^2 m_\pi^2}{f_\pi^4} \frac{\ell(\ell+1) + 2 - J(J+1)}{2\ell+1} \\ & \times \{ Q_{W,0}^{\ell-1}(k'_1, k_1) - Q_{W,0}^{\ell+1}(k'_1, k_1) - W_{\ell s,0}^\ell(k'_1, k_1) \} \end{aligned} \quad (11)$$

for the orbital and total angular momenta ℓ and J . The functions $Q_{W,0}^\ell$ and $W_{\ell s,0}^\ell$ are defined as

$$Q_{W,0}^\ell(k'_1, k_1) \equiv \frac{2\pi}{(2\pi)^3} \frac{1}{2} \int_0^{k_F} dk_3 Q_\ell(x') Q_\ell(x), \quad (12)$$

$$\begin{aligned}
W_{\ell s,0}^{\ell}(k'_1, k_1) &\equiv \frac{2\pi}{(2\pi)^3} \frac{1}{2k'_1 k_1} \int_0^{k_F} dk_3 k_3 \\
&\times \{k'_1 Q_{\ell}(x)[Q_{\ell-1}(x') - Q_{\ell+1}(x')] \\
&+ k_1 Q_{\ell}(x')[Q_{\ell-1}(x) - Q_{\ell+1}(x)]\}, \quad (13)
\end{aligned}$$

$$\begin{aligned}
\delta_{S1} \frac{c_3 g_A^2}{2f_{\pi}^4} \frac{\ell(\ell+1)+2-J(J+1)}{2\ell+1} &\left[\left[m_{\pi}^2 + \frac{1}{2}(k_1'^2 + k_1^2) \right] \{ Q_{W,0}^{\ell-1}(k'_1, k_1) - Q_{W,0}^{\ell+1}(k'_1, k_1) - W_{\ell s,0}^{\ell}(k'_1, k_1) \} \right. \\
&+ 3k'_1 k_1 \left\{ Q_{W,0}^{\ell}(k'_1, k_1) - (\ell-1)Q_{W,0}^{\ell-2}(k'_1, k_1) + (\ell+2)Q_{W,0}^{\ell+2}(k'_1, k_1) + \frac{\ell-1}{2\ell-1} W_{\ell s,0}^{\ell-1}(k'_1, k_1) + \frac{\ell+2}{2\ell+3} W_{\ell s,0}^{\ell+1}(k'_1, k_1) \right\} \\
&\left. - \delta_{\ell 1} \frac{k'_1 k_1}{2} (F_0(k'_1) + F_0(k_1) - F_1(k'_1) - F_1(k_1)) \right], \quad (14)
\end{aligned}$$

where the new functions $F_0(k)$ and $F_1(k)$ are defined as

$$F_0(k) \equiv \frac{1}{(2\pi)^3} \int \int \int_{|k_3| \leq k_F} dk_3 \frac{1}{(\mathbf{k} - \mathbf{k}_3)^2 + m_{\pi}^2}, \quad (15)$$

$$F_1(k) \equiv \frac{1}{(2\pi)^3} \frac{1}{k^2} \int \int \int_{|k_3| \leq k_F} dk_3 \frac{\mathbf{k} \cdot \mathbf{k}_3}{(\mathbf{k} - \mathbf{k}_3)^2 + m_{\pi}^2}. \quad (16)$$

Adding the reduced two-nucleon interaction to the Ch-EFT two-nucleon interaction, we repeat the LOBT G -matrix calculation. Although this paper gives explicit expressions for only the spin-orbit part, we include all the central, tensor, and spin-orbit components of the reduced interaction $v_{12(3)}$. The form factor with a functional form of $f(k'_1, k_1) = \exp\{-[(k'_1/\Lambda)^4 + (k_1/\Lambda)^4]\}$ is introduced for $v_{12(3)}$ with the cutoff mass $\Lambda = 550$ MeV. We use the low-energy constants fixed for the Jülich Ch-EFT potential given by Hebeler *et al.* [19]; $c_D = -4.381$ and $c_E = -1.126$. Other constants are $c_1 = -0.81$ GeV $^{-1}$, $c_3 = -3.4$ GeV $^{-1}$, and $c_4 = 3.4$ GeV $^{-1}$. Because the reduction of the 3NF to the two-nucleon force was performed in nuclear matter, $v_{12(3)}$ may not be directly applied to very light nuclei, such as ${}^3\text{H}$ and ${}^4\text{He}$.

We first comment on the calculated saturation curves given in Fig. 1. Without the contribution of the 3NF, the saturation curve attains its minimum at a larger Fermi momentum k_F than the empirical saturation momentum, as is already known. Nucleon-nucleon interactions, AV18 [20], NSC97 [21], and Jülich N 3 LO with a cutoff mass of 550 MeV [22], give similar saturation curves and the CD-Bonn potential [23] predicts somewhat deeper binding. To indicate which saturation curve is preferable for nuclear mean-field calculations, we also show the result for the Gogny D1S interaction [12].

The thin dotted curve shows the result obtained by adding the plane wave expectation value of the 3NF v_{123} to the result of the two-nucleon N 3 LO. The thick dotted curve next to the thin dotted curve is the result for the plane wave expectation value of the reduced two-nucleon interaction $v_{12(3)}$. The difference between these two curves originates from the difference in the form factors and the necessary approximation $\mathbf{k}'_1 + \mathbf{k}'_2 = \mathbf{k}_1 + \mathbf{k}_2 = 0$ in Eq. (8).

where $Q_{\ell}(x)$ is the Legendre function of the second kind, and $x' \equiv \frac{k_3^2 + k_1'^2 + m_{\pi}^2}{2k'_1 k_3}$ and $x \equiv \frac{k_3^2 + k_1^2 + m_{\pi}^2}{2k_1 k_3}$.

The spin-orbit component also originates from the c_3 term of the Ch-EFT 3NF. In this case, in addition to replacing the coupling constant, an additional factor $(\mathbf{k}'_1 - \mathbf{k}_3) \cdot (\mathbf{k}_3 - \mathbf{k}_1)$ appears in the denominator in Eq. (10). The partial-wave decomposition is given by

The solid curve is the result of the G -matrix calculation that includes the reduced two-nucleon interaction, $v_{12(3)}$. Although the energy is underestimated by a few million electron volts, the saturation properties are significantly improved by the repulsive contribution from the three-nucleon force. It is currently not necessary to realize perfect agreement with the empirical properties in the LOBT calculation in nuclear matter.

We now examine the spin-orbit strength. We tabulate, in Table I, values of $B_S(\bar{q})$ in Eq. (6) at $\bar{q} = 0.7$ fm $^{-1}$ calculated in the LOBT with modern nucleon-nucleon interactions: AV18 [20], NSC97 [21], CD-Bonn [23], and Jülich N 3 LO [22]. The Scheerbaum factors obtained by realistic two-nucleon forces are similar but insufficient to explain the spin-orbit strength required in nuclear mean-field calculations. Specifically, only about three fourths of the empirically required strength is

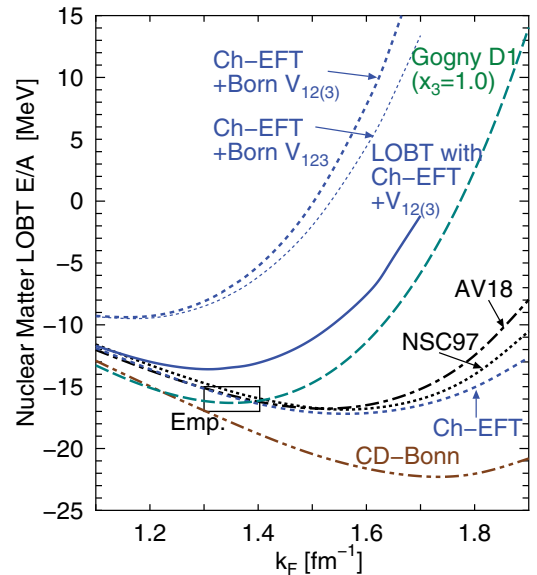


FIG. 1. (Color online) Saturation curves in symmetric nuclear matter.

accounted for. The two-body part of the Ch-EFT, $N^3\text{LO}$, differs little from other realistic two-nucleon forces. The values at $k_F = 1.07 \text{ fm}^{-1}$, namely at half of the normal density, vary little from those at the normal density with $k_F = 1.35 \text{ fm}^{-1}$. The last column in Table I shows that the addition of the reduced two-body interaction from the Ch-EFT 3NF reduces the discrepancy, although the 3NF contribution is smaller at $k_F = 1.07 \text{ fm}^{-1}$. This is consistent with the important role of the 3NF in spin-orbit splitting demonstrated in quantum Monte Carlo calculations of low-energy neutron- α scattering [24] by using the conventional 3NF in Ref. [5]. Although there are ambiguities from the form factor and uncertainties inherent in the folding procedure that do not account for nucleon-nucleon correlations, no additional adjustable parameters exist because low-energy constants c_1 and c_3 , which contribute solely to the spin-orbit strength, are determined in the two-nucleon sector.

As noted after Eq. (10), the reduced two-body spin-orbit term in neutron matter is one third that in symmetric nuclear matter. Actual G -matrix calculations using the Ch-EFT $N^3\text{LO}$ plus $v_{12(3)}$ in pure neutron matter with $k_F^n = 1.35 \text{ fm}^{-1}$ give $B_S(\bar{q})$ values at $\bar{q} = 0.7 \text{ fm}^{-1}$ of 84.7 and 93.5 MeV fm^5 without and with the reduced two-nucleon interaction $v_{12(3)}$, respectively. If $k_F^n = 1.07 \text{ fm}^{-1}$ is assumed, the corresponding values are 87.0 and 94.6 MeV fm^5 , respectively. Again, the k_F^n dependence is weak. While the spin-orbit strength from the two-nucleon force differs little from that in symmetric nuclear matter, the additional contribution from the three-nucleon force is almost one third that in symmetric nuclear matter. Thus, the spin-orbit strength is expected to be smaller in a neutron-rich environment. This seems to be consistent with the trend observed in the shell structure near the neutron

drip line [25], namely that the weaker spin-orbit interaction is preferable in the neutron excess region.

In summary, we have quantitatively estimated the contribution of the three-nucleon force of chiral effective field theory to the single-particle spin-orbit strength using the formulation of Scheerbaum [9]. We first introduced the reduced two-body interaction by folding the single-nucleon degrees of freedom of the 3NF in nuclear matter that includes the necessary statistical factor of $\frac{1}{3}$. Performing a partial-wave expansion of the resulting two-body interaction and adding it to the genuine two-nucleon interaction, we performed LOBT G -matrix calculations in infinite matter and evaluated the Scheerbaum factor corresponding to the spin-orbit strength. The detailed procedure of the partial wave decomposition that includes central and tensor components will be reported in a separate paper. Because the spin-orbit field in atomic nuclei is fundamentally important, as indicated by the nuclear magic numbers, it is important to know that including the 3NF in chiral effective field theory can account for the spin-orbit strength required for nuclear mean field calculations. Because the relevant low-energy constants, c_1 and c_3 , are determined in the two-nucleon interaction sector, there should be little uncertainty in the additional spin-orbit strength except for the treatment of the two-body form factor. The additional spin-orbit strength from the 3NF should be weaker in neutron-excess nuclei.

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