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SPIN OBSERVABLES AND PATH INTEGRALS

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Abstract

We discuss the formulation of spin observables associated to a non-relativistic spinning particles in terms of grassmanian differential operators. We use as configuration space variables for the pseudo-classical description of this system the positions x and a Grassmanian vector $\vec{\epsilon}$. We consider an explicit discretization procedure to obtain the quantum amplitudes as path integrals in this superspace. We compute the quantum action necessary for this description including an explicit expression for the boundary terms. Finally we shown how for simple examples, the path integral may be performed in the semi-classical approximation, leading to the correct quantum propagator.

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1 Introduction

The path integral [1] formulation of the quantum mechanics of fermionic systems is usually associated with the introduction of Grassmann variables [2] as pseudoclassical configuration variables (Nevertheless see Ref. [3] for an alternative approach in the relativistic case). The path integral treatment of a single fermionic degree of freedom is very well understood but, surprisingly, the extension of the formalism to a space time description of relativistic and non relativistic spinning particles or to the solution of potential problems has not been developed yet. Several approaches [2] using different sets of Grassmannian non-commuting variables have been proposed in the literature allowing to construct a pseudo-classical description of the dynamics of the spinning particle, (or pseudomechanics [4]) for the non-relativistic case, and for the Dirac electron [5] but this is not enough for a quantum description. With the pseudo-classical action identified, in order to write down a path integral expression for the fermionic propagator, it is necessary to construct an explicit representation of the spin observables and the polarized states of the particle in the Hilbert space associated to the Grassmann variables. This will we done in what follows. On the other hand, in the usual approach, [4] [5] this obstacle is bypassed by showing, instead that the constraint which emerge from imposing a variational principle to the action functional is equivalent in the operatorial formalism to the wave equation.Then the form of the propagator is borrowed from this formalism. This strategy, although enlightening from the conceptual point of view is not useful for computational purposes. Another path integral formalism, which is based on the use of Grassmannian coherent states [6], has been devised for the description of fermionic systems. It allows the computation of the propagator and bound state energies but the relation of this formalism with the pseudo-classical description is not completely clear and in particular does not provide a direct interpretation of the path integral as a sum over histories in configuration space. In what follows we also discuss how we can get this interpretation for spinning particles. First, we show that with an explicit realization of the spin observables one can represent the spin polarized states in the Grassmannian sector of the superspace. Then we derive the path integral formulation of the non-relativistic electron as a sum over histories directly from the pseudo-classical description. Finally, we show that being careful with the boundary conditions of the Grassmann functions one is able to compute the probability amplitudes using a semiclassical expansion.

2 Wave functions and spin observables

Consider a real Grassmannian vector $\vec{\epsilon}$ satisfying the anti-conmutation relations,

$$\epsilon_i \epsilon_j = -\epsilon_j \epsilon_i$$

and the super-configuration space of coordinates ($\vec{x}$,$\vec{\epsilon}$). Let us consider wave functions of both $\vec{x}$ and $\vec{\epsilon}$ with the general expansion ,

$$\phi(x, \vec{\epsilon}) = \phi(x) + \phi_i(x)\epsilon_i + \phi_{ij}(x)\epsilon_i\epsilon_j + \phi_{ijk}(x)\epsilon_i\epsilon_j\epsilon_k. \tag{1}$$

The functions $\phi_{ij}(x)$ and ϕ_{ijk} are anti-symmetric. The wave functions belong to a 8-dimensional complex vectorial space, ($\mathbb{C}^8$). The internal product in this space may be defined by,

$$\langle \phi_1 | \phi_2 \rangle = \int d\epsilon_3 d\epsilon_2 d\epsilon_1 (\phi^\dagger) I_\epsilon \phi_2. \tag{2}$$

where $d\epsilon_3 d\epsilon_2 d\epsilon_1$ is the Berezin integration measure. The operator I_ϵ is,

$$I_\epsilon = \frac{\epsilon_{ijk}}{3!} \left(\epsilon_i + \partial_i\right) \left(\epsilon_j + \partial_j\right) \left(\epsilon_k + \partial_k\right). \tag{3}$$

and $\partial_m = \frac{\partial}{\partial \epsilon_m}$ are the Grassmannian right derivatives which satisfy, $\partial_m \epsilon_k = \delta_{mk}$ and $\partial_m \epsilon_k \epsilon_j = \delta_{mk}\epsilon_j - \delta_{mj}\epsilon_k$. If one considers the eight independent functions in ϕ as the components of a vector in ($\mathbb{C}^8$), the internal product defined in (2) corresponds to the usual product in ($\mathbb{C}^8$). The δ function in the odd sector is given by

$$\delta(\vec{\epsilon}' - \vec{\epsilon}) = \left(\epsilon'_1 - \epsilon_1\right) \left(\epsilon'_2 - \epsilon_2\right) \left(\epsilon'_3 - \epsilon_3\right). \tag{4}$$

Introduce the non-Hermitian position operator E in the odd sector of the configuration space and the continuous set of eigenvectors $|\vec{\epsilon}\rangle$ of E. Similarly as in the coherent state representation we have the relations

$$\langle \vec{\epsilon} | \vec{\epsilon}' \rangle = e^{\vec{\epsilon}' . \vec{\epsilon}}. \tag{5}$$

An arbitrary wave function $\phi(x,\epsilon_i)$ is represented in Dirac notation in the form, $\phi(x,\epsilon_i) = \langle\vec{x},\vec{\epsilon}|\phi\rangle$. The identity operator in the odd sector is

$$\mathbb{1} = \int d\epsilon_3 d\epsilon_2 d\epsilon_1 |\vec{\epsilon}'\rangle I_\epsilon \langle\vec{\epsilon}|, \tag{6}$$

and we note also that, $I_\epsilon e^{\epsilon'\epsilon} = \delta(\epsilon - \epsilon')$. The physical sector of this space should be expanded by the spin polarized states. To represent the spin observables $\vec{S}$ we introduce the differential operators,

$$S_i = -\frac{i}{4}\epsilon_{ijk}\left(\epsilon_j + \partial_j\right)\left(\epsilon_k + \partial_k\right) \tag{7}$$

which satisfy the angular momentum algebra, $[S_i, S_j] = i\epsilon_{ijk}S_k$. This representation of the spin observables is the natural generalization of the usual representation of the fermionic position-momentum algebra which led to the coherent state formulation of the path integral[7]. It has been discussed also in Ref. [8]. Looking at things from another point of view, the Hilbert space of states $|\vec{\epsilon}\rangle$ and the operators (7) provide a fermionic coherent state representation of the $SU(2)$ algebra alternative to the bosonic approach [9]. This construction may be generalized to other groups. The complete set of eigenfunctions of S_3 is given in the following table.

f^n_λ	λ	$\phi(\vec{\epsilon})$
f^1_+	$\frac{1}{2}$	$1 - i\epsilon_1\epsilon_2$
f^2_+	$\frac{1}{2}$	$\epsilon_3 - i\epsilon_1\epsilon_2\epsilon_3$
f^3_+	$\frac{1}{2}$	$\epsilon_1 + i\epsilon_2$
f^4_+	$\frac{1}{2}$	$-\epsilon_1\epsilon_3 - i\epsilon_2\epsilon_3$
f^4_-	$-\frac{1}{2}$	$1 + i\epsilon_1\epsilon_2$
f^3_-	$-\frac{1}{2}$	$\epsilon_3 + i\epsilon_1\epsilon_2\epsilon_3$
f^2_-	$-\frac{1}{2}$	$\epsilon_1 - i\epsilon_2$
f^1_-	$-\frac{1}{2}$	$-\epsilon_1\epsilon_3 + i\epsilon_2\epsilon_3$

The eigenvalues of S_3, denoted by λ are which, as can be seen, degenerate. To construct a particular base of states, we take a linear combination of them in such a way that the action of the up and down operators $S_+ = S_1 + iS_2$ and $S_- = S_1 - iS_2$ is well defined. A possible choice of the eigenfunctions which represent the polarized states is

$$\begin{aligned} \langle\vec{\epsilon}|+\rangle &= (1+\epsilon_3)(1 - i\epsilon_1\epsilon_2), \\ \langle\vec{\epsilon}|-\rangle &= (1-\epsilon_3)(\epsilon_1 - i\epsilon_2). \end{aligned} \tag{8}$$

3 The action functional and the path integral

Let us consider now a spinning particle whose dynamics is determined by the Hamiltonian operator H. We want to discuss a discretization procedure in the trajectories of the particle in the configuration space which allows to represent the Green functions in terms of a path integral. The evolution operator is given by,

$$U(t_f - t_i) = e^{-iH(t_f - t_i)}. \tag{9}$$

with matrix elements, $U(x, \vec{\epsilon}, t; x', \vec{\epsilon}', t') = \langle x', \vec{\epsilon}' | U(t, t') | x, \vec{\epsilon} \rangle$. For the spin polarized states ($k = +, -$), we define the physical propagator, $K(k, t_f; j, t_i = \langle x_f, k | U | x_i, j \rangle$ which may be projected in the form,

$$K(k, t_f; j, t_i) = \int d\epsilon_i \int d\epsilon_f \langle k | \epsilon_f \rangle I_{\epsilon_f} \langle \epsilon_f | U(x_f, \epsilon_f, t_f; x_i, \epsilon_i, t_i) | \epsilon_i \rangle I_{\epsilon_i} \langle \epsilon_i | j \rangle. \tag{10}$$

(we drop the arrow on the Grassmann coordinates).Now consider a discretization $\{t_1, t_2, \ldots, t_{2N}\}$ with $\delta = t_k - t_{k-1}$ of the time interval, and using the resolution of unity let us compute the matrix element of the evolution operator. We get,

$$\begin{aligned}
&\langle x_f, \epsilon_f | e^{-iH(t_f - t_i)} | x_i, \epsilon_i \rangle = \\
&\lim_{2N \to \infty} \int \Pi_{k=1}^{\infty} \frac{dp_k}{2\pi} \int \Pi_{j=1}^{\infty} dx_j \int d\epsilon_1' \int d\epsilon_1 \int d\epsilon_2' \int d\epsilon_2 \ldots \int d\epsilon_{2N}' \int d\epsilon_{2N} \\
&\langle x_f, \epsilon_f || p_{2N}, \epsilon_{2N} \rangle I_{\epsilon_{2N}} \langle p_{2N}, \epsilon_{2N} | e^{-iH\delta} | x_{2N}, \epsilon_{2N}' \rangle I_{\epsilon_{2N}'} \langle x_{2N}, \epsilon_{2N}' | \ldots \\
&\ldots \langle \epsilon_k, p_k | e^{-iH\delta} | x_k, \epsilon_k' \rangle I_{\epsilon_k'} \langle x_k, \epsilon_k' || p_{k-1}, \epsilon_{k-1} \rangle I_{\epsilon_{k-1}} \langle p_{k-1}, \epsilon_{k-1} | \ldots \\
&\ldots \langle \epsilon_1, p_1 | e^{-iH\delta} | x_1, \epsilon_1' \rangle I_{\epsilon_1'} \langle x_1, \epsilon_1' | x_i, \epsilon_i \rangle.
\end{aligned}$$

The general term can be expanded in the form,

$$\begin{aligned}
&I_{\epsilon_k} \langle \epsilon_k, p_k | e^{-iH\delta} | x_k, \epsilon_k' \rangle I_{\epsilon_k'} \langle x_k, \epsilon_k' | p_{k-1}, \epsilon_{k-1} \rangle = \\
&I_{\epsilon_k'} e^{-iH(p_k, x_k, \epsilon_k)\delta} e^{-ip_k x_k} e^{\epsilon_k' \epsilon_k} I_{\epsilon_k'} e^{ip_{k-1} x_{k-1}} e^{\epsilon_{k-1} \epsilon_k'} = \\
&e^{-iH_0(p_k, x_k)\delta} e^{-ip_k x_k} e^{ip_{k-1} x_{k-1}} I_{\epsilon_k'} e^{-iH_1(x_k, \epsilon_k)\delta} e^{\epsilon_k' \epsilon_k} I_{\epsilon_k'} e^{\epsilon_{k-1} \epsilon_k'}
\end{aligned}$$

were we use that the hamiltonian function satisfies,

$$H(p_k, x_k, \epsilon_k) = H_0(p_k, x_k) + H_1(x_k, \epsilon_k). \tag{11}$$

This is obvious if H does not depend on the ϵ derivatives, but it is also true in the general case due to the external integrals. Let us focus in the Grassmann sector alone and note that under the integral sign we have,

$$
\begin{aligned}
&\langle\epsilon_f|\epsilon_{2N}\rangle I_{\epsilon_{2N}} e^{-iH_1(x_{2N},\epsilon_{2N})\delta} e^{\epsilon'_{2N}\epsilon_{2N}} I_{\epsilon'_{2N}} e^{\epsilon_{2N-1}\epsilon'_{2N}} \ldots I_{\epsilon_1} e^{-iH_1(x_1,\epsilon_1)\delta} e^{\epsilon_i\epsilon_1} = \\
&e^{\frac{1}{2}\epsilon_{2N}\epsilon_f} e^{-iH(p_{2N},x_{2N},\epsilon_{2N})\delta+\frac{1}{2}\epsilon_{2N}\left(\epsilon_f-\epsilon_{2N-1}\right)} e^{-iH(p_{2N-1},x_{2N-1},\epsilon_{2N-1})\delta+\frac{1}{2}\epsilon_{2N-1}(\epsilon_{2N}-\epsilon_{2N-2})} \ldots \\
&e^{-iH(p_1,x_1,\epsilon_1)\delta+\frac{1}{2}\epsilon_1(\epsilon_2-\epsilon_i)} e^{\frac{1}{2}\epsilon_i\epsilon_1}.
\end{aligned}
$$

The terms at the end of the interval are of the form,

$$
\begin{aligned}
\vec{\epsilon}_{2N}\vec{\epsilon}_f &\approx (\vec{\epsilon}_f - \delta\dot{\vec{\epsilon}}_f)\vec{\epsilon}_f = \delta\vec{\epsilon}_f\dot{\vec{\epsilon}}_f, && (12)\\
\vec{\epsilon}_i\vec{\epsilon}_1 &\approx \vec{\epsilon}_i(\vec{\epsilon}_i + \delta\dot{\vec{\epsilon}}_i) = \delta\vec{\epsilon}_i\dot{\vec{\epsilon}}_i. && (13)
\end{aligned}
$$

In the limit $2N \to \infty$ ($\delta \to 0$), they reduce to boundary terms which depend only of initial and final values

$$
g(\vec{\epsilon}_i, \vec{\epsilon}_f) = \lim_{\delta\to 0} \frac{1}{2}\left\{\int_{t_i}^{t_i+\delta} \vec{\epsilon}\dot{\vec{\epsilon}}dt + \int_{t_f-\delta}^{t_f} \vec{\epsilon}\dot{\vec{\epsilon}}dt\right\}. \tag{14}
$$

Incorporating the bosonic sector we are left with,

$$
U(\vec{\epsilon}_f, t_f; \vec{\epsilon}_i, t_i) = \int D[\epsilon]D[x]D[p]e^{g(\vec{\epsilon}_i,\vec{\epsilon}_f)+i\int\left\{\dot{\vec{x}}\vec{p}-\frac{i\vec{\epsilon}\dot{\vec{\epsilon}}}{2}-H(x,p,\epsilon)\right\}dt}. \tag{15}
$$

The action functional recovered in the measure of the path integral is the one that appears in the pseudoclassical description of the spinning particle [4]. To compute the quantum ampitude between physical states, one introduces (15) in (10).

4 The semiclassical approximation and the variational principle

Bosonic path integrals with quadratic potentials may be computed using a semiclassical approximation [1]. In this section we show that a similar result holds also in the case under consideration if proper care is given to the boundary terms. The point here is that, since the equations for $\vec{\epsilon}$ are first order, it is not possible in general to find trajectories $x(t)$ and $\vec{\epsilon}(t)$, extremals of S in the time interval $t_f - t_i$, with $x(t_i) = x_i$, $x(t_f) = x_f$, $\epsilon(t_i) = \epsilon_i$ and $\epsilon(t_f) = \epsilon_f$. So we introduce two Lagrange multipliers π_i, π_f and consider instead an extended action

$$S^*[\epsilon(t), \pi_i, \pi_f] = S[\epsilon(t)] + \pi_i(\epsilon(t_i) - \epsilon_i) - \pi_f(\epsilon(t_f) - \epsilon_f). \tag{16}$$

The equations of motion are

$$2\left(\left(\frac{\partial L}{\partial \dot{\epsilon}}\right)(t_f) - \pi_f\right)\delta(t - t_f) - 2\left(\left(\frac{\partial L}{\partial \dot{\epsilon}}\right)(t_i) - \pi_i\right)\delta(t - t_i) = 0, \tag{17}$$
$$x(t_i) = x_i, x(t_f) = x_f.$$

Now we can fix the values of the Lagrange multipliers to guarantee that the boundary conditions, which here appear as independent equations, are satisfied. In fact, we still have the freedom to fix π_i to zero. Then the solution to the equations may be written in the form

$$\vec{\epsilon}_{class} = \vec{\epsilon_0} + \vec{\delta_\epsilon}\Theta(t - t_f) \tag{18}$$

where $\vec{\epsilon_0}$ satisfies

$$\dot{\vec{\epsilon_0}} = i\frac{\partial H}{\partial \vec{\epsilon_0}}. \tag{19}$$

and δ_ϵ is a jump at the end of the trajectory. To perform the semiclassical expansion let us consider first the free case with the action given by,

$$iS = g(\vec{\epsilon_i}, \vec{\epsilon_f}) + i\int\left[-\frac{i\vec{\epsilon}\dot{\vec{\epsilon}}}{2}\right]dt. \tag{20}$$

The solution to the equations of motion which satisfies the boundary condition is simply

$$\vec{\epsilon}(t) = \vec{\epsilon_i} + 2(\vec{\epsilon_f} - \vec{\epsilon_i})\Theta(t - t_f). \tag{21}$$

Consider the path integral (15) computed in the previous section with the boundary term (14), and let us perform an expansion around $\vec{\epsilon}_{class}$,

$$\vec{\epsilon}(t) = \vec{\epsilon}_{class}(t) + \vec{\xi}(t). \tag{22}$$

Substituting (22) and (21) in (15) we get the expected result,

$$U(\vec{\epsilon_f}, t_f; \vec{\epsilon_i}, t_i) = Ne^{\epsilon_i\epsilon_f}. \tag{23}$$

Let us turn out our attention to a more general case. The most general even Hamiltonian function has the form,

$$H(x,p,\epsilon) = H_0(x,p) + H_{ij}(x)\epsilon_i\epsilon_j. \tag{24}$$

Then, the equation of motion is linear in ϵ. Using the equation of motion for ϵ_0, and the linearity of the equation of motion it is readily seen that the boundary term takes the form,

$$g(\vec{\epsilon}_i,\vec{\epsilon}_f) = \frac{\vec{\epsilon}_0(t_f)\vec{\epsilon}_f}{2}. \tag{25}$$

This result generalizes for the interacting case the expression obtained by Galvao and Teitelboim [4]. Consider again expressions of the form (22) and (22). Substitution in (15) leads us to the expression,

$$g(\vec{\epsilon}_i,\vec{\epsilon}_f) + iS = \vec{\epsilon}_0(t_f)\vec{\epsilon}_f + \tag{26}$$
$$i\int_{t_i}^{t_f} dt \left\{ \left[-i\frac{\vec{\epsilon}_0\dot{\vec{\epsilon}}_0}{2} + H_0(x,p) + H_{ij}\epsilon_{0i}\epsilon_{0j} \right] + \left[-\frac{i}{2}\vec{\xi}\dot{\vec{\xi}} + H_{ij}\xi_i\xi_j \right] \ldots \right\}$$

for the exponent. (The dots appear to denote possible bosonic contributions). Then, in the case when the spin degrees of freedom factorize, we get the following simple expression for the matrix elements

$$U(\vec{\epsilon}_f,t_f;\vec{\epsilon}_i,t_i) = Ne^{2g(\vec{\epsilon}_f,\vec{\epsilon}_i)}. \tag{27}$$

where N is a normalizacion constant.

5 Spin precession

Let us recover the known results for particle in a uniform magnetic field for example. The action is given by

$$S = g(\vec{\epsilon}_i,\vec{\epsilon}_f) + \int \left(\dot{\vec{x}}\vec{p} - \frac{i}{2}\vec{\epsilon}\dot{\vec{\epsilon}} + \frac{p^2}{2m} + \frac{q}{2m}\left(\frac{\epsilon_{ijk}}{2} i\epsilon_j\epsilon_k\right) B_i \right) dt. \tag{28}$$

Defining,

$$M_{jk} = \frac{q}{2m}\frac{\epsilon_{ijk}}{2}B_i, \tag{29}$$

we are left with the Lagrangian,

$$L = -\frac{i\vec{\epsilon}\dot{\vec{\epsilon}}}{2} + i\frac{\vec{\epsilon}^T M\vec{\epsilon}}{2}. \tag{30}$$

The equation of motion is simply, $\dot{\vec{\epsilon}}_0(t) = M\vec{\epsilon}_0(t)$, and the classical trajectory with arbitrary boundary conditions is given by,

$$\begin{aligned} \vec{\epsilon}_{class}(t) &= e^{M(t-t_i)}\vec{\epsilon}_i + \vec{\delta}_\epsilon \Theta(t-t_f), \\ \dot{\vec{\epsilon}}_{class}(t) &= Me^{M(t-t_i)}\vec{\epsilon}_i + \vec{\delta}_\epsilon \delta(t-t_f), \end{aligned} \tag{31}$$

Defining $\omega = \frac{qB}{m}$ we have,

$$e^{M(t-t_i)} = \begin{pmatrix} cos(\omega(t-t_i)) & sen(\omega(t-t_i)) & 0 \\ -sen(\omega(t-t_i)) & cos(\omega(t-t_i)) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{32}$$

In this case the boundary term $g(\vec{\epsilon}_f, \vec{\epsilon}_i)$ is nontrivial and takes the form

$$g(\vec{\epsilon}_f, \vec{\epsilon}_i) = \frac{\vec{\epsilon}_i^t e^{-M(t_f-t_i)}\vec{\epsilon}_f}{2}. \tag{33}$$

According with the discussion of the previous section the we have now,

$$U(\vec{\epsilon}_f, t_f; \vec{\epsilon}_i, t_i) = e^{\vec{\epsilon}_i^t e^{-M(t_f-t_i)}\vec{\epsilon}_f}. \tag{34}$$

To recover the standard result we compute the time evolution of an arbitrary wave function

$$\phi(\vec{\epsilon}_f, t_f) = \int d\epsilon_i I_{\vec{\epsilon}_f} e^{\vec{\epsilon}_i^t e^{-M(t_f-t_i)}\vec{\epsilon}_f}\phi(\vec{\epsilon}_i, t_i) = \phi(e^{-M(t_f-t_i)}\vec{\epsilon}_f, t_i). \tag{35}$$

With the initial state, $|\phi_i\rangle = cos(\frac{\theta}{2})e^{\frac{-i\varphi}{2}}|+\rangle + sen(\frac{\theta}{2})e^{\frac{i\varphi}{2}}|-\rangle$ and $\vec{B}$ directed in the x_3 direction, we get

$$\begin{aligned} \langle\phi(t)|S_3|\phi(t)\rangle &= cos(\theta), \\ \langle\phi(t)|S_1|\phi(t)\rangle &= sen(\theta)cos(\varphi+\omega t), \\ \langle\phi(t)|S_2|\phi(t)\rangle &= sen(\theta)sen(\varphi+\omega t). \end{aligned} \tag{36}$$

6 Conclusion

In this paper we have assembled many sparse elements of the the theory of spinning particle already found in the literature, and developed a little some of them, to construct a path integral representation of the quantum amplitudes of a non-relativistic electron in an external electromagnetic field. This fermionic path integral shares the interpretation of a sum over (pseudo) classical histories with its bosonic counterpart. The clue in this approach is to build up the path integral from the explicit realization of the spin operators. The main technical point in the computations concerns the correct handling of the boundary contributions. There are various natural ways to develop further the work presented in this paper. First, one can extend the computational techniques to cases where the spin and the translational degrees of freedom are mixed by the interaction (For example in Ref.[10]). One can also generalize this approach to the relativistic Dirac particle as we discuss elsewhere [11]. Finally the relation between the Grassmannian representation of the spin observables and the fermionic $SU(2)$ coherent states may be generalized for other groups.

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