Resonating mean-field theoretical approach to the Nambu–Jona-Lasinio model

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Using the Nambu–Jona-Lasinio (NJL) model, the dynamical chiral-symmetry breaking, the light-mesons spectra, and the properties of the mesons have been investigated on the basis of a conventional Hartree-Fock approach. In order to show the advantage of the resonating (Res) mean-field theory for a fermion system with large quantum fluctuations over the usual mean-field theory, we apply it to the NJL model to describe more precisely such phenomena associated with the pionic excitation. For the sake of simplicity, a state with large quantum fluctuations is approximated by the superposition of two Dirac seas, namely nonorthogonal Slater determinants (S-dets) with different correlation structures. We consider two cases: in the first case both Dirac seas are composed of *equal* ''constituent quark masses'' while in the second case the constituent quark masses are *unequal*. We make a direct optimization of the Res-mean-field energy functional, i.e., a variation of the Res-mean-field ground-state energy with respect to the Res-mean-field parameters, the ''constituent quark masses.'' Then the Res-mean-field ground and excited states generated with the S-dets explain most of a mass spectrum and associated properties of the pion. [S0556-2813(99)05811-2]

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I. INTRODUCTION

In transitional nuclei, resonances between different superconducting states with small deformations, and between different deformed states with large deformations having nearly degenerate energies, are known to arise. The effects of such resonances becomes important at the lower end of superdeformed bands, where a transition to the ground-state minimum occurs. This effect reflects the importance of quantum fluctuations. It is the advantage of microscopic investigations that there are methods at hand to go to beyond the mean-field theory and to take these quantum fluctuations into account. Fukutome and one of the present authors (S.N.) have proposed theories called the resonating Hartree-Fock (Res-HF) theory [1] and the resonating Hartree-Bogoliubov (Res-HB) theory [2] to treat the problem of large quantum fluctuations in normal fermion systems and superconducting fermion systems.

A fermion system with small quantum fluctuations can be described by a standard method of fermion many-body theory, namely the mean-field theory. The ground state of the system is well approximated by a single determinantal HF or HB mean-field wave function. Quantum fluctuations can be taken into account as zero-point oscillations of a time-dependent mean field with small amplitudes around the minimum in the energy functional surface. Such fluctuations and collective excitations connected with them can be treated by the well-known random-phase approximation (RPA). If the quantum fluctuations around the mean field become large and so the energy functional has a large anharmonicity in its low-energy portion, then nonlinear couplings between the RPA excitation modes, the so-called mode-mode couplings, become important. When the anharmonicity in the energy functional surface increases so much that the surface has multiple low-energy minima, the approximation by a single mean-field wave function is certainly no longer possible and the RPA also breaks down.

In the Res-HF and Res-HB theories, the ground state is assumed to become a superposition of multiple mean-field wave functions, namely to be resonating between different correlation structures. The first application of the Res-HB theory was made to the problem of describing the resonance of multiple shapes coexistence in nuclei by using a simple model with strong pairing correlations [3]. The Res-HF theory has been applied to a well-known exactly solvable model in order to clarify some essential features of the theory and to show its advantage over the usual HF theory. In this study, the Res-HF ground state with a few Slater determinants (S-dets) reproduces the exact ground-state energy and explains most of the ground-state correlation energy in all the correlation regimes [4–6]. Then it has turned out that the Res-HF approximation is a promising tool and provides a method to work better than the usual HF. Very recently, the Res-mean-field theory has also been successfully applied by one of the present authors (S.N.) [7] to a resonating relativistic mean-field description of exotic phenomena in nuclei, in the spirit of the relativistic mean-field approach.

Quantum chromodynamics (QCD) is now widely recognized as the fundamental theory of strong interactions. In QCD, spontaneous breaking of chiral symmetry, leading to a condensate of quark-antiquark pairs in the QCD vacuum, plays a crucial role in the description of low-energy characteristics of hadrons. The quark-antiquark condensation caused by dynamical chiral-symmetry breaking was proposed by Nambu and Jona-Lasinio (NJL) in 1961 [8]. The NJL model, which contains a chiral effective interaction between quarks (the four-fermion interaction), has been shown to provide a framework for the spontaneous realization of chiral-symmetry breaking and allows for the collective mesonic excitations whose properties have the characteristics of

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physical particles. The NJL model has been regarded as a reasonable approximation to QCD for intermediate length scales. The context of the original NJL model has been accepted as a manageable approximation to dynamical chiral-symmetry breaking because it has the advantage of being easier to handle than QCD itself. Then in this context the problem of a deeper understanding of mechanism of chiral-symmetry breaking arises naturally as well as its consequences for the low-energy properties of hadrons, namely the spectra and the properties of the light mesons.

Using the NJL model Hamiltonian, one of the present authors (J. da P.), Ruivo, and Sousa have investigated dynamical chiral-symmetry breaking, light-mesons spectra and properties of the mesons on the basis of the conventional HF and time-dependent HF (TDHF) approaches [9]. This theoretical framework and technique in many-body problems, very familiar to nuclear physicists, turned out to be appropriate to describe the properties of hadrons in an exceedingly intuitive way in the spirit of a mean-field approximation. The HF procedure describes the realization of a stable equilibrium configuration in the context of the mean-field approximation in the sense that a vacuum expectation value of the Hamiltonian takes a minimal value. The TDHF method gives RPA collective excitations with small amplitudes which allow to interpret both the low-energy light-mesons mass spectra and properties of the mesons [10–12].

The Res-mean-field theories are able to treat in a rigorous manner large quantum fluctuations and strong correlation effects due to quantum- and dynamical-tunneling effects falling outside the scope of the RPA and of mode-mode coupling theories. Of course, they can also deal with small quantum fluctuations which are describable by the usual RPA. Thus, they have a possibility to reveal surprisingly dramatic aspects of the physics of fermion systems with large quantum fluctuations. The Res-mean-field methods have been constructed on the basis of a group-theoretical deduction starting from the fact that they are based, in their group-theoretical backgrounds, on the Lie algebras of the fermion pair operators arising from the canonical anticommutation relation of the fermion. Therefore, from the above-mentioned reasons, they should have a universal applicability to problems of current topics in wider fields of physics. The radical spirit of the Res-mean-field theory may be expected to open a new field also for the exploration of the low-energy hadron physics taking notice of the strong analogy between a chiral effective Hamiltonian with a four-fermion interaction and a familiar nonrelativistic fermion Hamiltonian with a two-body force.

In order to investigate the advantage of the Res-mean-field theory over the usual mean-field theory, we apply it to the naive NJL model without isospin [8] to describe more precisely such phenomena of the pion mentioned previously. For the sake of simplicity, a state with large quantum fluctuations is approximated by the superposition of two Dirac seas, namely nonorthogonal S-dets with different correlation structures. We consider two cases: in the first case both Dirac seas are composed of *equal* ‘‘constituent quark masses,’’ while in the second, the constituent quark masses are *unequal*. We make a direct optimization of the Res-mean-field energy functionals, i.e., a variation of the Res-mean-field ground-state energy with respect to the Res-mean-field parameters, namely the ‘‘constituent quark masses.’’ Our final objective is to explain the mass spectrum and associated properties of the pion by the Res-mean-field ground and excited states generated with the two S-dets.

Along the above lines this paper is organized as follows. In Sec. II we present the naive NJL model and a brief recapitulation of the resonating mean-field approximation. In Sec. III we consider only two S-dets with different correlation structures having *equal* constituent quark masses. We introduce isometric matrices in terms of components of a matrix induced by a Thouless transformation to get overlap integral, interstate density matrix and matrix element of the Hamiltonian between nonorthogonal S-dets. Instead of solving the Res-mean-field equations, we make a direct optimization of the Res-mean-field energy functional, i.e., a variation of the Res-mean-field ground-state energy. In Sec. IV we adopt two S-dets with different correlation structures with *unequal* constituent quark masses. In Sec. V we give a Res-mean-field ground-state energy and describe a collective excitation around the stable equilibrium vacuum which is interpreted as a pion mass spectrum. In Sec. VI we calculate an order parameter and a pion decay constant by using the self-consistent solution of the Res-mean-field equation. Finally, in Sec. VII, after discussing the behavior of the overlap integral in the Res-mean-field approximation of the NJL model, we give a summary and the concluding remarks. As might be expected, we find that the present numerical results are very similar to those of the previous works [10,12].

II. MODEL AND RESONATING MEAN-FIELD APPROXIMATION

We consider a naive NJL model which describes a system of many quarks interacting via a two-body force according to the chiral-invariant Hamiltonian

$$H=\sum_{i=1}^{N} \mathbf{p}_i \cdot \boldsymbol{\alpha}_i - g\sum_{i\neq j}^{N} \delta(\mathbf{r}_i-\mathbf{r}_j)[\beta_i\beta_j-\beta_i\gamma_i^5\beta_j\gamma_j^5], \tag{2.1}$$

where $\boldsymbol{\alpha}_i$, β_i, and γ_i^5 stand for the standard Dirac matrices acting on the degrees of freedom of the quark i and g is the coupling constant. Here we use the former version of the NJL model with only one single flavor but without isospin [8]. Following the work by one of the present authors (J. da. P.), Ruivo, and Sousa [9], when $g=0$, the above NJL Hamiltonian describes a massless Dirac free quark and a Dirac sea (the S-det) of massless quark having zero chirality is given as

$$|\Phi_0\rangle=\prod_{i=1}^{N} d_i^{\dagger(0)}|0\rangle, \tag{2.2}$$

where $d_i^{\dagger(0)}$ is the creation operator of a massless negative-energy state and $|0\rangle$ is the absolute vacuum. The index i stands for the momentum $\mathbf{p}$ and helicity s and the absolute value of $\mathbf{p}_i$ satisfies $|\mathbf{p}_i|\leqslant\Lambda$ (the highest momentum of the occupied states). When g is switched on, the system undergoes a phase transition into a state of chiral broken symmetry above a critical value of the coupling strength $g_{\rm cr}$. As the consequence of the chiral-symmetry breaking, the nonzero constituent quark mass M is produced dynamically: namely, the quarks acquire a dynamical mass. A Dirac sea (the S-det) of massive quarks is written as

$$|\Phi\rangle=\prod_{i=1}^{N} d_i^\dagger|0\rangle, \tag{2.3}$$

where $d_i^\dagger$ is the creation operator of a massive negative-energy state. According to Refs. [8, 9], the operators b_i ($b_i^\dagger$) and d_i ($d_i^\dagger$) are related to $b_i^{(0)}$ ($b_i^{\dagger(0)}$) and $d_i^{(0)}$ ($d_i^{\dagger(0)}$) by means of the canonical transformation

$$\begin{aligned}[b_{-\mathbf{p},s},b_{\mathbf{p},s},d^\dagger_{-\mathbf{p},s},d^\dagger_{\mathbf{p},s}]&=U(g)[b^{(0)}_{-\mathbf{p},s},b^{(0)}_{\mathbf{p},s},d^{\dagger(0)}_{-\mathbf{p},s},d^{\dagger(0)}_{\mathbf{p},s}]U^\dagger(g)\\&=[b^{(0)}_{-\mathbf{p},s},b^{(0)}_{\mathbf{p},s},d^{\dagger(0)}_{-\mathbf{p},s},d^{\dagger(0)}_{\mathbf{p},s}]g.\end{aligned} \tag{2.4}$$

The $U(g)$ is a unitary operator to induce a Thouless transformation [13] and the 4×4 matrix g is given as

$$\begin{aligned}g&=\sqrt{\frac{1+\beta_\mathbf{p}}{2}}\cdot I+\sqrt{\frac{1-\beta_\mathbf{p}}{2}}\cdot\gamma^5\beta\Sigma_1,\\ gg^\dagger&=g^\dagger g=I_4,\quad \det g=1,\end{aligned} \tag{2.5}$$

where $\beta_\mathbf{p}=|\mathbf{p}|/E_\mathbf{p}$ and $E_\mathbf{p}=\sqrt{\mathbf{p}^2+M^2}$. By $\det g$ we denote the determinant of the matrix g. By I_4 we denote the four dimensional unit matrix and by Σ_1 the first component of the 4×4 matrix-valued vector $\mathbf{\Sigma}=(\Sigma_1,\Sigma_2,\Sigma_3)$ which is represented as

$$\mathbf{\Sigma}=\begin{bmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{bmatrix},\quad \boldsymbol{\sigma}=(\sigma_1,\sigma_2,\sigma_3), \tag{2.6}$$

where $\boldsymbol{\sigma}$ denotes the vector having the Pauli matrices for components. In the Res-mean-field approximation, the constituent quark mass M is treated as a variational parameter. The total number of quarks in the negative-energy states is N and a momentum cutoff Λ is used in order to regularize the Res-mean-field theory [9].

Following Fukutome [1], we give here a brief recapitulation of the resonating mean-field approximation. We consider an n-fermion system with N single-particle states. Let a_i and $a_i^\dagger$, $i=1,2,...,N$, be the annihilation and creation operators of the fermion, and let the Hamiltonian of the system be

$$H=h_{ji}a_j^\dagger a_i+\frac{1}{4}[ki|lj]a_k^\dagger a_l^\dagger a_j a_i, \tag{2.7}$$

where h_{ij} and $[ki|lj]$ denote the single-particle Hamiltonian and the antisymmetrized interaction-matrix elements, respectively. Here and hereafter we use the summation convention over repeated indices unless the possibility of misunderstanding arises.

A wave function $|\Psi\rangle$ is exactly represented in an integral form as

$$\begin{aligned}|\Psi\rangle&={}_NC_n\int U(g)|\phi\rangle\langle\phi|U^\dagger(g)|\Psi\rangle dg\\&={}_NC_n\int |g\rangle\langle g|\Psi\rangle dg,\end{aligned} \tag{2.8}$$

and the Schrödinger equation $(H-E)|\Psi\rangle=0$ can be converted into an integral equation

$$\int \{H[W(g,g')]-E\}\langle g|g'\rangle\Psi(g')dg'=0, \tag{2.9}$$

where the integration is the group integration over a unitary group U(N) of N dimension made of a unitary matrix g corresponding to coefficients of linear combinations of the fermions. The state $|\Psi\rangle$ is a coherent-state representation (CS rep) of fermion state vectors represented by a function $\Psi(g)=\langle g|\Psi\rangle$ on U(N). The ket $|g\rangle$ is given as $|g\rangle=U(g)|\phi\rangle$ in which the unitary operator $U(g)$ induces a Thouless transformation of a reference S-det $|\phi\rangle$ [13]. The U(N) CS rep of n particle state is a representation on the coset U(N)/U(n) denoted as u which is an $N\times n$ submatrix of a U(N) matrix. The Hamiltonian matrix element and overlap integral between two nonorthogonal S-dets $|u\rangle$ and $|u'\rangle$ are given as

$$\begin{aligned}\langle u|H|u'\rangle&=H[W(u,u')]\langle u|u'\rangle,\quad \langle u|u'\rangle=\det z,\\ z&=u^\dagger u',\end{aligned} \tag{2.10}$$

where z is an $n\times n$ matrix and $\det z$ is the determinant of z. The interstate density matrix $W(u,u')$ is defined as

$$W(u,u')=u'z^{-1}u^\dagger, \tag{2.11}$$

which is an $N\times N$ dimensional matrix and satisfies

$$W(u,u')=W^2(u,u'),\quad W^\dagger(u,u')=W(u',u). \tag{2.12}$$

This reduces to the usual mean-field density matrix if $u=u'$.

We approximate $|\Psi\rangle$ by a discrete superposition of S-dets as

$$|\Psi\rangle=\sum_f |u_f\rangle c_f. \tag{2.13}$$

We denote sampling S-dets as $|u_f\rangle$. The mixing coefficients c_f are normalized by

$$\langle\Psi|\Psi\rangle=\sum_{f,f'}\langle u_f|u_{f'}\rangle c_f^* f_{f'}=\sum_{f,f'}\det z_{ff'}c_f^*c_{f'}=1, \tag{2.14}$$

where $z_{ff'}=u_f^\dagger u_{f'}=z_{f'f}^\dagger$.

The expectation value of the Hamiltonian H (2.7) in $|\Psi\rangle$ is expressed as

$$\langle\Psi|H|\Psi\rangle=\sum_{f,f'}\langle u_f|H|u_{f'}\rangle c_f^* c_{f'} =\sum_{f,f'} H[W_{ff'}]\det z_{ff'} c_f^* c_{f'}, \quad (2.15)$$

$$H[W_{ff'}]=h_{ji}(W_{ff'})_{ij}+\frac{1}{2}[ki|lj](W_{ff'})_{ik}(W_{ff'})_{jl}, \quad (2.16)$$

where $W_{ff'}=u_{f'}z_{ff'}^{-1}u_f^\dagger$ is the interstate density matrix between $|u_f\rangle$ and $|u_{f'}\rangle$.

We determine both the c_f and $|u_f\rangle$ variationally by the following set of equations:

$$\sum_{f'}(H[W_{ff'}]-E)\det z_{ff'}c_{f'}=0, \quad (2.17)$$

$$\sum_{f'}K_{ff'}c_f^* c_{f'}=0, \quad (2.18)$$

where

$$K_{ff'}=\{(1-W_{ff'})F[W_{ff'}]+H[W_{ff'}]-E\}W_{ff'}\cdot\det z_{ff'}. \quad (2.19)$$

Equation (2.17) is called the Res-mean-field configuration-interaction (CI) equation. Optimization of the orbitals u_f is made by Eq. (2.18) which we call the Res-mean-field equation. The $N\times N$ matrix-valued Res-mean-field interstate Fock operator $F_{ij}[W_{ff'}]$ is given through the functional derivative of the Hamiltonian matrix element as

$$F_{ij}[W_{ff'}]=\frac{\delta H[W_{ff'}]}{\delta(W_{ff'})_{ji}}=h_{ij}+[ij|kl](W_{ff'})_{lk}. \quad (2.20)$$

The Res-mean-field interstate Fock operator reduces to the usual Fock operator if the sampling S-dets are restricted to only one S-det.

III. RESONATING MEAN-FIELD EQUATION WITH EQUAL CONSTITUENT QUARK MASSES

Any S-det$|\Phi(g)\rangle(=|g\rangle)$ can be constructed by the action of $U(g)$ given by Eq. (2.4) on a reference S-det$|\Phi_0\rangle$, Eq. (2.2), (the Thouless theorem [13]) as

$$|g\rangle=U(g)|\Phi_0\rangle =\prod_{\mathbf{p},s}\left(\frac{1+\beta_{\mathbf{p}}}{2}\right)\exp\left(\sum_{\mathbf{p},s}\sqrt{\frac{1-\beta_{\mathbf{p}}}{1+\beta_{\mathbf{p}}}}b_{\mathbf{p},s}^{\dagger(0)}d_{\mathbf{p},s}^{(0)}\right)|\Phi_0\rangle, \quad (3.1)$$

which means that the S-det of massive quarks in the negative-energy states may be written as a coherent superposition of massless quark-antiquark pairs in the negative-energy states. The constituent quark mass M is generated as the result of the dynamical chiral-symmetry breaking of the system [9].

For simplicity, we here consider only two S-dets corresponding to the usual mean-field states of two local energy minima with different correlation structures having *equal* constituent quark masses M. We denote them as $|g_1\rangle$ and $|g_2\rangle$. They are distinguished by writing explicitly the subscripts 1 and 2 [5].

In order to get the explicit expression for the Res-mean-field equation, we must calculate the overlap integral $\det z_{12}$, the interstate density matrix $W(u_1,u_2)$, the matrix element of the Hamiltonian $\langle u_1|H|u_2\rangle$ and the interstate Fock operator $F[W(u_1,u_2)]$ between nonorthogonal S-dets. For this aim, we introduce two 4×2 isometric matrices $u_{1,\mathbf{p},r}$ and $u_{2,\mathbf{p},r}$ and a 2×2 matrix $z_{12,\mathbf{p}}$ by

$$u_{1,\mathbf{p},r}=\begin{bmatrix}-\sqrt{\dfrac{1-\beta_{\mathbf{p}}}{2}}\boldsymbol{\sigma}\cdot\mathbf{n}\cdot\chi_r\\ \sqrt{\dfrac{1+\beta_{\mathbf{p}}}{2}}\cdot\chi_r\end{bmatrix}, \quad u_{2,\mathbf{p},r}=\gamma^5 u_{1,\mathbf{p},r} \quad (r=1,2), \quad (3.2)$$

$$\chi_1=\begin{bmatrix}1\\0\end{bmatrix}, \quad \chi_2=\begin{bmatrix}0\\1\end{bmatrix}, \quad (3.3)$$

$$u_{1(2),\mathbf{p},r}^\dagger u_{1(2),\mathbf{p},r'}=\delta_{rr'}, \quad (r,r'=1,2), \qquad z_{12,\mathbf{p},rr'}=u_{1,\mathbf{p},r}^\dagger u_{2,\mathbf{p},r'}, \quad (3.4)$$

where $\mathbf{n}$ is the unit vector for components. Substituting Eq. (3.2) into the second equation of Eq. (3.4), we have

$$z_{12,\mathbf{p},rr'}=-\frac{1}{E_{\mathbf{p}}}\chi_r^\dagger\boldsymbol{\sigma}\cdot\mathbf{p}\chi_{r'}, \quad (r,r'=1,2), \quad (3.5)$$

from which explicit forms of the matrix and the inverse matrix together with the determinantal value of the $z_{12,\mathbf{p},rr'}$ are obtained as

$$z_{12,\mathbf{p}}=-\frac{1}{E_{\mathbf{p}}}\boldsymbol{\sigma}\cdot\mathbf{p}, \quad z_{12,\mathbf{p}}^{-1}=-\frac{E_{\mathbf{p}}}{\mathbf{p}^2}\boldsymbol{\sigma}\cdot\mathbf{p}, \quad \det z_{12,\mathbf{p}}=-\frac{\mathbf{p}^2}{E_{\mathbf{p}}^2}. \quad (3.6)$$

Then the overlap integral $\det z_{12}$ is calculated as

$$\det z_{12}=\prod_{\mathbf{p}}\det z_{12,\mathbf{p}}\theta(\Lambda^2-p^2) =\exp\left(\sum_{\mathbf{p}}(\ln\det z_{12,\mathbf{p}})\theta(\Lambda^2-p^2)\right) =\exp\left[a\left(\ln\frac{1}{1+x^2}-2x^2+2x^3\tan^{-1}\frac{1}{x}\right)\right], \quad x\equiv\frac{M}{\Lambda}, \quad (3.7)$$

where we have used $\Sigma_{\mathbf{p}}=V\int d^3\mathbf{p}/(2\pi)^3$ and $V=6\pi^2 a/\Lambda^3$ (a is the dimensionless volume parameter). Here, we had to introduce the dimensionless volume parameter a to get a finite value of the overlap integral $\det z_{12}$. It may be interpreted that the a gives a confinement volume of quarks, i.e., a volume of a space in which the quarks are confined. It is in general agreed that the main drawback of the NJL model is the lack of confinement. It is known that the NJL vacuum is unstable. The NJL vacuum associated with a chiral rotation $e^{iB\gamma^5 z}$ of the NJL Hamiltonian may have indeed a lower energy than the original vacuum. This deficiency may be a manifestation of the lack of confinement. Some sort of stabilizing mechanism may be indeed required [14]. The use of a confinement volume, as in the present calculation, is a possible choice. The step function θ is defined as

$$\theta(x)=\begin{cases}1, & x\geqslant 0,\\ 0, & x<0.\end{cases}$$

The usual mean-field density matrices $W_{11,\mathbf{p}}$ and $W_{22,\mathbf{p}}$ for the negative-energy state and the interstate density matrix $W_{12,\mathbf{p}}$ are calculated as

$$W_{11,\mathbf{p}}=\sum_{r=1}^{2} u_{1,\mathbf{p},r}u^{\dagger}_{1,\mathbf{p},r}=\frac{1}{2}\left(1-\frac{\mathbf{p}\cdot\boldsymbol{\alpha}+\beta M}{\sqrt{\mathbf{p}^2+M^2}}\right)\theta(\Lambda^2-p^2), \tag{3.8}$$

$$W_{22,\mathbf{p}}=\sum_{r=1}^{2} u_{2,\mathbf{p},r}u^{\dagger}_{2,\mathbf{p},r} =\frac{1}{2}\left(1-\frac{\mathbf{p}\cdot\boldsymbol{\alpha}-\beta M}{\sqrt{\mathbf{p}^2+M^2}}\right)\theta(\Lambda^2-p^2)=\gamma^5 W_{11,\mathbf{p}}\gamma^5, \tag{3.9}$$

$$W_{12,\mathbf{p}}=\sum_{r,r'=1}^{2} u_{2,\mathbf{p},r}(z^{-1}_{12,\mathbf{p}})_{rr'}u^{\dagger}_{1,\mathbf{p},r'} =\frac{1}{2}\left(1-\frac{\mathbf{p}\cdot\boldsymbol{\alpha}(E_{\mathbf{p}}-\beta M)}{\mathbf{p}^2}\right)\theta(\Lambda^2-p^2). \tag{3.10}$$

To get the correct density matrix $W_{11,\mathbf{p}}$ for the negative-energy state given in Ref. [9], we have replaced $\beta_{\mathbf{p}}=|\mathbf{p}|/E_{\mathbf{p}}$ with $\beta_{\mathbf{p}}=M/E_{\mathbf{p}}$ in Eq. (3.2). The interstate density matrix $W_{12,\mathbf{p}}$ obviously satisfies the idempotency condition but is not Hermitian.

The usual mean-field energy functional $\langle u_1|H|u_1\rangle$ $(=H[W_{11}])$ has already been obtained in Ref. [9] and expressed as

$$H[W_{11}]=-\frac{1}{4\pi^2}\Lambda^4\left[\sqrt{1+x^2}-\frac{3}{2}x^2 v(x)+\frac{g\Lambda^2}{\pi^2}x^2v^2(x)+\frac{2}{9}\frac{g\Lambda^2}{\pi^2}\right]V, \tag{3.11}$$

where $v(x)\equiv\sqrt{1+x^2}-x^2\ln f(x)$ and $f(x)\equiv 1/x+\sqrt{1+1/x^2}$. Owing to the property of the density matrix $W_{22,\mathbf{p}}=\gamma^5 W_{11,\mathbf{p}}\gamma^5$, Eq. (3.9), the mean-field energy functional $\langle u_2|H|u_2\rangle(=H[W_{22}])$ is simply expressed as

$$H[W_{22}]=H[W_{11}]. \tag{3.12}$$

This important result means that the S-dets $|u_1\rangle$ and $|u_2\rangle$ have degenerate energies but different correlation structures with each other. By using the explicit form for the interstate density matrix $W_{12,\mathbf{p}}$ Eq. (3.10), the matrix element of the Hamiltonian $\langle u_1|H|u_2\rangle$ can be easily calculated as

$$\langle u_1|H|u_2\rangle=H[W_{12}]\cdot\det z_{12},$$

$$H[W_{12}]=-\frac{1}{4\pi^2}\Lambda^4\left[\sqrt{1+x^2}+\frac{1}{2}x^2v(x)+\frac{2}{9}\frac{g\Lambda^2}{\pi^2}\right]V, \tag{3.13}$$

detailed computation of which is given in the appendixes.

The Res-mean-field configuration-interaction (CI) equation to determine the mixing coefficients c_1 and c_2 is written simply in terms of the real quantities as follows:

$$\begin{bmatrix} H[W_{11}]-E & (H[W_{12}]-E)\cdot\det z_{12}\\ (H[W_{12}]-E)\cdot\det z_{12} & H[W_{22}]-E\end{bmatrix}\begin{bmatrix}c_1\\ c_2\end{bmatrix}=0, \tag{3.14}$$

together with the normalization condition

$$c_1^2+c_2^2+2c_1c_2\det z_{12}=1. \tag{3.15}$$

Due to the relation $H[W_{11}]=H[W_{22}]$, Eq. (3.12), which we denote simply as $H[W]$, we can get the Res-mean-field energy E and the corresponding magnitudes of the mixing coefficients c_1 and c_2 as follows:

$$E=\frac{1}{1-(\det z_{12})^2}\{H[W]-H[W_{12}](\det z_{12})^2 \mp|H[W]-H[W_{12}]|\det z_{12}\},$$

$$c_1^2=c_2^2=\left(1+\frac{(H[W]-E)^2}{(H[W_{12}]-E)^2(\det z_{12})^2}-2\frac{H[W]-E}{H[W_{12}]-E}\right)^{-1}. \tag{3.16}$$

Then the Res-mean-field energy E is classified into the following two kinds of solutions:

$$\text{case I:}\quad H[W]-H[W_{12}]>0,$$

$$E_{\mathrm{g}}^{\mathrm{Res}}=\frac{1}{1+\det z_{12}}(H[W]+H[W_{12}]\cdot\det z_{12}),$$

$$E_{\mathrm{ex}}^{\mathrm{Res}}=\frac{1}{1-\det z_{12}}(H[W]-H[W_{12}]\cdot\det z_{12}), \tag{3.17}$$

$$\text{case II:} \quad H[W]-H[W_{12}]<0,$$

$$E_{\text{gr}}^{\text{Res}}=\frac{1}{1-\det z_{12}}(H[W]-H[W_{12}]\cdot\det z_{12}),$$

$$E_{\text{ex}}^{\text{Res}}=\frac{1}{1+\det z_{12}}(H[W]+H[W_{12}]\cdot\det z_{12}). \quad (3.18)$$

It should be stressed that the Res-mean-field energies and the corresponding mixing coefficients must be determined so as to optimize the energy expectation value by the superposed wave function $c_1|u_1\rangle+c_2|u_2\rangle$.

Instead of solving the Res-mean-field equations $\Sigma_{f=1}^{2}K_{1f}c_1^*c_f=0$ and $\Sigma_{f=1}^{2}K_{2f}c_2^*c_f=0$, we here make a direct optimization of the Res-mean-field energy functional. This is easily achieved by a variation of the Res-mean-field ground-state energy $E_{\text{gr}}^{\text{Res}}$ with respect to the Res-mean-field variational parameter x,

$$\frac{d}{dx}E_{\text{gr}}^{\text{Res}}=0, \quad (3.19)$$

which leads to

$$\frac{d}{dx}H[W](1+\det z_{12})+\frac{d}{dx}H[W_{12}]\cdot\det z_{12}(1+\det z_{12}) -(H[W]-H[W_{12}])\frac{d}{dx}\det z_{12}=0 \quad (\text{for case I}), \quad (3.20)$$

$$\frac{d}{dx}H[W](1-\det z_{12})-\frac{d}{dx}H[W_{12}]\cdot\det z_{12}(1-\det z_{12}) +(H[W]-H[W_{12}])\frac{d}{dx}\det z_{12}=0 \quad (\text{for case II}). \quad (3.21)$$

These are the self-consistency conditions for cases I and II, respectively, in the Res-mean-field approximation. The similarity between the self-consistency conditions and the so called ''gap equation'' in the BCS theory [15,16] and in the Res-HB theory [2,3] is a manifestation of the analogy of the present Res-mean-field theory with the BCS theory which motivated the NJL model [8]. Substituting the differential formulas for the diagonal and off-diagonal matrix elements of the Hamiltonian

$$\frac{d}{dx}H[W]=-\frac{1}{4\pi^2}\Lambda^4\cdot 6x\left[\frac{g\Lambda^2}{\pi^2}v(x)-1\right] \times\left[v(x)-\frac{2}{3}\frac{1}{\sqrt{1+x^2}}\right]V, \quad (3.22)$$

$$\frac{d}{dx}H[W_{12}]=-\frac{1}{4\pi^2}\Lambda^4\cdot 2xv(x)V, \quad (3.23)$$

into Eqs. (3.20) and (3.21), we can get the following formulas connecting the coupling constant g with the variational parameter x for both cases I and II

$$\frac{g\Lambda^2}{\pi^2}=\frac{1}{v(x)\left[v(x)-\frac{2}{3}\frac{1}{\sqrt{1+x^2}}\right](1+\det z_{12})-\frac{1}{6}xv^2(x)\frac{d}{dx}\det z_{12}}\left\{\left(v(x)-\frac{2}{3}\frac{1}{\sqrt{1+x^2}}\right)(1+\det z_{12}) -\frac{1}{3}v(x)\det z_{12}(1+\det z_{12})-\frac{1}{3}xv(x)\frac{d}{dx}\det z_{12}\right\} \quad (\text{for case I}) \quad (3.24)$$

$$\frac{g\Lambda^2}{\pi^2}=\frac{1}{v(x)\left[v(x)-\frac{2}{3}\frac{1}{\sqrt{1+x^2}}\right](1-\det z_{12})+\frac{1}{6}xv^2(x)\frac{d}{dx}\det z_{12}}\left\{\left(v(x)-\frac{2}{3}\frac{1}{\sqrt{1+x^2}}\right)(1-\det z_{12}) +\frac{1}{3}v(x)\det z_{12}z_2(1-\det z_{12})+\frac{1}{3}xv(x)\frac{d}{dx}\det z_{12}\right\} \quad (\text{for case II}), \quad (3.25)$$

where the differential of the overlap integral is given by

$$\frac{d}{dx}\det z_{12}=-6ax\left(1-x\tan^{-1}\frac{1}{x}\right)\cdot\det z_{12}. \quad (3.26)$$

It is easily seen that Eqs. (3.24) and (3.25) just coincide with the result in Ref. [9] if we set $\det z_{12}=0$. It turns out that the occurrence of the relations (3.24) and (3.25) of the coupling constant to the variational parameter is attributed to the consequence of taking quantum- and dynamical-tunneling effects into account.

IV. RESONATING MEAN-FIELD EQUATION WITH UNEQUAL CONSTITUENT QUARK MASSES

We are now in a stage to superpose the S-dets with *unequal* constituent quark masses M_1 and M_2. Along the same line as in Sec. III, we introduce two 4×2 isometric matrices $u_{1,1\mathbf{p},r}$ and $u_{2,2\mathbf{p},r}$ and a 2×2 matrix $z_{12,\mathbf{p}}$ by

$$u_{1,1\mathbf{p},r}=\begin{bmatrix} -\sqrt{\dfrac{1-\beta_{1\mathbf{p}}}{2}}\,\boldsymbol{\sigma}\cdot\mathbf{n}\cdot\chi_r \\ \sqrt{\dfrac{1+\beta_{1\mathbf{p}}}{2}}\cdot\chi_r \end{bmatrix},\quad u_{2,2\mathbf{p},r}=\gamma^5 u_{1,2\mathbf{p},r}\quad (r=1,2), \tag{4.1}$$

$$u^{\dagger}_{1(2),1(2)\mathbf{p},r}u_{1(2),1(2)\mathbf{p},r'}=\delta_{rr'}\quad (r,r'=1,2),\quad z_{12,\mathbf{p},rr'}=u^{\dagger}_{1,1\mathbf{p},r}u_{2,2\mathbf{p},r'}\,. \tag{4.2}$$

Substituting Eq. (4.1) into Eq. (4.2), we have

$$z_{12,\mathbf{p},rr'}=-\frac{1}{2}\left(\sqrt{1-\beta_{1\mathbf{p}}}\sqrt{1+\beta_{2\mathbf{p}}}+\sqrt{1+\beta_{1\mathbf{p}}}\sqrt{1-\beta_{2\mathbf{p}}}\right)\chi_r^{\dagger}\boldsymbol{\sigma}\cdot\mathbf{p}\chi_{r'}\,,\quad (r,r'=1,2), \tag{4.3}$$

where $\beta_{1(2)\mathbf{p}}=M_{1(2)}/E_{1(2)\mathbf{p}}$ and $E_{1(2)\mathbf{p}}=\sqrt{\mathbf{p}^2+M^2_{1(2)}}$. From Eq. (4.3) explicit forms of the matrix and the inverse matrix together with the determinantal value of the $z_{12,\mathbf{p},rr'}$ are obtained as

$$z_{12,\mathbf{p}}=-\frac{1}{\tilde{E}_{\mathbf{p}}}\boldsymbol{\sigma}\cdot\mathbf{p},\quad z^{-1}_{12,\mathbf{p}}=-\frac{\tilde{E}_{\mathbf{p}}}{\mathbf{p}^2}\boldsymbol{\sigma}\cdot\mathbf{p},\quad \det z_{12,\mathbf{p}}=-\frac{1}{2}\left(1+\frac{\mathbf{p}^2-M_1M_2}{E_{1\mathbf{p}}E_{2\mathbf{p}}}\right), \tag{4.4}$$

where

$$\tilde{E}_{\mathbf{p}}=\frac{2\sqrt{E_{1\mathbf{p}}}\sqrt{E_{2\mathbf{p}}}}{\sqrt{E_{1\mathbf{p}}/p-M_1/p}\sqrt{E_{2\mathbf{p}}/p+M_2/p}+\sqrt{E_{1\mathbf{p}}/p+M_1/p}\sqrt{E_{2\mathbf{p}}/p-M_2/p}}. \tag{4.5}$$

Then the overlap integral $\det z_{12}$ is calculated as

$$\det z_{12}=\prod_{\mathbf{p}}\det z_{12,\mathbf{p}}\theta(\Lambda^2-p^2)=\exp\left(\sum_{\mathbf{p}}(\ln\det z_{12,\mathbf{p}})\,\theta(\Lambda^2-p^2)\right)=\exp[az(x_1,x_2)],\quad x_1\equiv\frac{M_1}{\Lambda},\quad x_2\equiv\frac{M_2}{\Lambda}. \tag{4.6}$$

The function $z(x_1,x_2)$ is given as

$$\begin{aligned}z(x_1,x_2)={}&\frac{1}{3}-\ln 2-(x_1^2+x_2^2)+\left(x_1^3\tan^{-1}\frac{1}{x_1}+x_2^3\tan^{-1}\frac{1}{x_2}\right)+\ln\left(1+\frac{1-x_1x_2}{\sqrt{1+x_1^2}\sqrt{1+x_2^2}}\right)-\frac{1}{3}(1-2x_1^2+3x_1x_2-x_2^2)\sqrt{\frac{1+x_1^2}{1+x_2^2}}\\&-\frac{1}{3}x_1(2x_1^2-3x_1x_2+2x_2^2)E\left(\tan^{-1}\frac{1}{x_2},\sqrt{1-\frac{x_2^2}{x_1^2}}\right)+\frac{1}{3}x_1x_2^2F\left(\tan^{-1}\frac{1}{x_2},\sqrt{1-\frac{x_2^2}{x_1^2}}\right),\quad (x_1\geqslant x_2)\end{aligned} \tag{4.7}$$

$$\begin{aligned}z(x_1,x_2)={}&\frac{1}{3}-\ln 2-(x_2^2+x_1^2)+\left(x_2^3\tan^{-1}\frac{1}{x_2}+x_1^3\tan^{-1}\frac{1}{x_1}\right)+\ln\left(1+\frac{1-x_2x_1}{\sqrt{1+x_2^2}\sqrt{1+x_1^2}}\right)-\frac{1}{3}(1-2x_2^2+3x_2x_1-x_1^2)\sqrt{\frac{1+x_2^2}{1+x_1^2}}\\&-\frac{1}{3}x_2(2x_2^2-3x_2x_1+2x_1^2)E\left(\tan^{-1}\frac{1}{x_1},\sqrt{1-\frac{x_1^2}{x_2^2}}\right)+\frac{1}{3}x_2x_1^2F\left(\tan^{-1}\frac{1}{x_1},\sqrt{1-\frac{x_1^2}{x_2^2}}\right)\quad (x_2\geqslant x_1),\end{aligned} \tag{4.8}$$

where $E(\phi,k)$ and $F(\phi,k)$ are the Legendre's incomplete elliptic integral of the second kind and the incomplete elliptic integral of the first kind, respectively, and detailed computation of them are given in the appendixes [17]. By using the two isometric matrices (4.1) and the inverse matrix (4.4), the usual mean-field density matrices $W_{11,\mathbf{p}}$ and $W_{22,\mathbf{p}}$ for the negative-energy states are shown to have essentially the same forms as those of Eqs. (3.8) and (3.9) and are given as

$$W_{11,\mathbf{p}}=\frac{1}{2}\left(1-\beta\frac{M_1}{E_{1\mathbf{p}}}-\gamma^5\frac{\mathbf{\Sigma}\cdot\mathbf{p}}{E_{1\mathbf{p}}}\right)\theta(\Lambda^2-p^2), \qquad (4.9)$$

$$W_{22,\mathbf{p}}=\frac{1}{2}\left(1+\beta\frac{M_2}{E_{2\mathbf{p}}}-\gamma^5\frac{\mathbf{\Sigma}\cdot\mathbf{p}}{E_{2\mathbf{p}}}\right)\theta(\Lambda^2-p^2)$$
$$=\gamma^5 W_{11,\mathbf{p}}(M_1\to M_2)\gamma^5, \qquad (4.10)$$

but the interstate density matrix $W_{12,\mathbf{p}}$ is shown to change drastically from Eq. (3.10) including a term proportional to β and is calculated as

$$W_{12,\mathbf{p}}=\frac{1}{2}\left(1+\beta\frac{A_\mathbf{p}-B_\mathbf{p}}{A_\mathbf{p}+B_\mathbf{p}}-\gamma^5\frac{C_\mathbf{p}+D_\mathbf{p}}{A_\mathbf{p}+B_\mathbf{p}}\mathbf{\Sigma}\cdot\mathbf{p}\right.$$
$$\left.-\beta\gamma^5\frac{C_\mathbf{p}-D_\mathbf{p}}{A_\mathbf{p}+B_\mathbf{p}}\mathbf{\Sigma}\cdot\mathbf{p}\right)\theta(\Lambda^2-p^2), \qquad (4.11)$$

where

$$A_\mathbf{p}\equiv\sqrt{E_{1\mathbf{p}}/p-M_1/p}\sqrt{E_{2\mathbf{p}}/p+M_2/p},$$

$$B_\mathbf{p}\equiv\sqrt{E_{1\mathbf{p}}/p+M_1/p}\sqrt{E_{2\mathbf{p}}/p-M_2/p},$$

$$C_\mathbf{p}\equiv\sqrt{E_{1\mathbf{p}}/p+M_1/p}\sqrt{E_{2\mathbf{p}}/p+M_2/p}\cdot\frac{1}{p},$$

$$D_\mathbf{p}\equiv\sqrt{E_{1\mathbf{p}}/p-M_1/p}\sqrt{E_{2\mathbf{p}}/p-M_2/p}\cdot\frac{1}{p}. \qquad (4.12)$$

The interstate density matrix $W_{12,\mathbf{p}}$ obviously satisfies the idempotency condition but is not Hermitian and just coincides with Eq. (3.10) if we set $M_1=M_2=M$.

As was already shown in Sec. III, the usual mean-field energy functionals $\langle u_1|H|u_1\rangle(=H[W_{11}])$ and $\langle u_2|H|u_2\rangle$ $(=H[W_{22}])$ are expressed as

$$H[W_{11}]=-\frac{1}{4\pi^2}\Lambda^4\left[\sqrt{1+x_1^2}-\frac{3}{2}x_1^2v(x_1)+\frac{g\Lambda^2}{\pi^2}x_1^2v^2(x_1)+\frac{2}{9}\frac{g\Lambda^2}{\pi^2}\right]V, \qquad (4.13)$$

$$H[W_{22}]=-\frac{1}{4\pi^2}\Lambda^4\left[\sqrt{1+x_2^2}-\frac{3}{2}x_2^2v(x_2)+\frac{g\Lambda^2}{\pi^2}x_2^2v^2(x_2)+\frac{2}{9}\frac{g\Lambda^2}{\pi^2}\right]V. \qquad (4.14)$$

By using the explicit form for the interstate density matrix $W_{12,\mathbf{p}}$, Eq. (4.11), the matrix element of the Hamiltonian $\langle u_1|H|u_2\rangle$ is easily calculated as

$$\langle u_1|H|u_2\rangle=H[W_{12}]\cdot\det z_{12},$$

$$H[W_{12}]=-\frac{1}{4\pi^2}\Lambda^4\left\{\frac{1}{x_1+x_2}\left[x_1\left(\sqrt{1+x_2^2}+\frac{1}{2}x_2^2v(x_2)\right)+x_2\left(\sqrt{1+x_1^2}+\frac{1}{2}x_1^2v(x_1)\right)\right]\right.$$
$$+\frac{1}{4}\frac{g\Lambda^2}{\pi^2}\frac{1}{(x_1+x_2)^2}\left[\sqrt{1+x_1^2}+\frac{1}{2}x_1^2v(x_1)-\sqrt{1+x_2^2}-\frac{1}{2}x_2^2v(x_2)\right]^2\left.+\frac{2}{9}\frac{g\Lambda^2}{\pi^2}\right\}V, \qquad (4.15)$$

detailed computation of which is given in the appendixes. This expression for the $\langle u_1|H|u_2\rangle$ reduces to that given by Eq. (3.13) if we set $x_1=x_2=x$.

By solving the Res-mean-field CI equation (3.14), we can get the Res-mean-field energy E and the corresponding magnitudes of the mixing coefficients c_1 and c_2 as follows:

$$E=\begin{bmatrix}E_{\rm gr}^{\rm Res}\\ E_{\rm ex}^{\rm Res}\end{bmatrix}$$
$$=\frac{1}{2-2(\det z_{12})^2}\{H[W_{11}]+H[W_{22}]-2H[W_{12}](\det z_{12})^2\mp\sqrt{E_{\rm dis}}\}, \qquad (4.16)$$

$$E_{\rm dis}\equiv(H[W_{11}]-H[W_{22}])^2+4(H[W_{11}]-H[W_{12}])\times(H[W_{22}]-H[W_{12}])(\det z_{12})^2, \qquad (4.17)$$

$$c_1^2=\left(1+\frac{(H[W_{11}]-E)^2}{(H[W_{12}]-E)^2(\det z_{12})^2}-2\frac{H[W_{11}]-E}{H[W_{12}]-E}\right)^{-1}, \qquad (4.18)$$

$$c_2^2=\left(1+\frac{(H[W_{22}]-E)^2}{(H[W_{12}]-E)^2(\det z_{12})^2}-2\frac{H[W_{22}]-E}{H[W_{12}]-E}\right)^{-1}. \qquad (4.19)$$

A direct optimization of the Res-mean-field energy functional is easily achieved by a variation of the Res-mean-field ground-state energy $E_{\rm gr}^{\rm Res}$ with respect to the Res-mean-field variational parameters x_1 and x_2,

$$\frac{\partial}{\partial x_1}E_{\rm gr}^{\rm Res}(x_1,x_2)=0, \quad \frac{\partial}{\partial x_2}E_{\rm gr}^{\rm Res}(x_1,x_2)=0, \qquad (4.20)$$

which leads us to

$$\frac{\partial}{\partial x_{1(2)}} H[W_{11(22)}]\{H[W_{11}]+H[W_{22}]-2H[W_{12}]-2(H[W_{22(11)}]-H[W_{12}])[1-(\det z_{12})^2]\}[1-(\det z_{12})^2]$$
$$-\frac{\partial}{\partial x_{1(2)}} H[W_{12}]2(H[W_{11}]+H[W_{22}]-2H[W_{12}])(\det z_{12})^2[1-(\det z_{12})^2]$$
$$+\{(H[W_{11}]+H[W_{22}]-2H[W_{12}])^2+E_{\rm dis}\}(\det z_{12})\frac{\partial}{\partial x_{1(2)}}\det z_{12}$$
$$=\Bigg\{2(H[W_{11}]+H[W_{22}]-2H[W_{12}])(\det z_{12})\frac{\partial}{\partial x_{1(2)}}\det z_{12}$$
$$+\left(\frac{\partial}{\partial x_{1(2)}}H[W_{11(22)}]-2\frac{\partial}{\partial x_{1(2)}}H[W_{12}](\det z_{12})^2\right)[1-(\det z_{12})^2]\Bigg\}\sqrt{E_{\rm dis}}, \quad (4.21)$$

where $(\partial/\partial x_{1(2)})H[W_{11(22)}]$ stands for $(\partial/\partial x_1)H[W_{11}]$ or $(\partial/\partial x_2)H[W_{22}]$, etc. The partial differentials of the $\det z_{12}$ are given in the appendixes.

V. RESONATING GROUND-STATE ENERGY AND PION MASS SPECTRUM

There are actually three parameters Λ (the cutoff parameter), g (the coupling constant), and a (the volume parameter) in the present NJL model. According to [10], however, in the present paper we use the value of the cutoff parameter $\Lambda=631.0$ MeV. First we solve numerically the resonating mean-field equation for *equal* constituent quark masses. The dimensionless quantity $g\Lambda^2$ for both cases I ($H[W]-H[W_{12}]>0$) and II ($H[W]-H[W_{12}]<0$) is plotted as a function of an inverse of the Res-mean-field variational parameter $1/x(=\Lambda/M)$ through Eqs. (3.24) and (3.25) for several values of the model parameter a. We show in Fig. 1 the behavior of the dimensionless quantity $g\Lambda^2$ plotted against Λ/M for several values of the dimensionless volume parameter a and compare with that of the conventional HF approach [9].

The behavior of the dimensionless quantity $g\Lambda^2$ for both cases I and II is very similar to that of the usual HF approach [9] if Λ/M is small. It, however, decreases rapidly as Λ/M becomes larger for case I and increases for case II though in the case of the usual HF approach it approaches $\pi^2(\simeq 9.87)$ as closely as possible, as indicated by the thick solid curve [9]. We can see that the behavior of the $g\Lambda^2$ for case II is quite opposite to that for case I. This tendency is more conspicuous as the dimensionless volume parameter a becomes smaller. The $g\Lambda^2$ well reproduces a reasonable value of the magnitude of the coupling constant g if the Λ/M is small. Let us investigate the signature of the energy difference $H[W]-H[W_{12}]$ for both cases I and II by using the $g\Lambda^2$ calculated through Eqs. (3.24) and (3.25). It is shown numerically that the energy difference is always positive for both cases I and II. Then for case II we have no physical solution. The value of the $g\Lambda^2/\pi^2$ for case I shows a gradual decrease as x and a become small and a slow increase to a position $\Lambda/M\simeq 3.0$ for $a=9$.

If we give a value of the constituent quark mass M, i.e., x, the quantity $g\Lambda^2$ is obtained and then the Res-mean-field ground- and excited- state energies for case I are determined through Eq. (3.17). In order to determine x, if we intend to solve the nonlinear equation (3.20) by using the simple iterative method, we would surely encounter a very serious problem of nonconvergence as we have often experienced in the usual HF and HB calculations. To avoid such a convergence difficulty, we will employ a direct-optimization method. For the purpose of constructing a tractable-optimization algorithm, let us introduce a quantity Δx which brings us the most effective change to decrease the value of the Res-mean-field ground-state energy $E_{\rm gr}^{\rm Res}$ at each iteration step. To get fast convergence the Res-mean-field quantity Δx must be determined so as to optimize the energy variation up to the second order. It is the quadratic steepest descent of the Res-mean-field ground-state energy $E_{\rm gr}^{\rm Res}$ with respect to the S-dets, $|u_1\rangle$ and $|u_2\rangle$ but with *equal* constituent quark masses M. Starting from a certain initial value of x, we cal culate the quadratic steepest descent Δx. We employ the calculated $x+\Delta x$ as the new trial value of x in the next iteration step. We must continue our Res-mean-field calculations by iterating in succession many time steps until convergence is achieved. Our numerical calculations are carried out at the region $g\Lambda^2=11.00$–15.50 and $a=3.00$–7.50. If the value of either $g\Lambda^2$ or a become large, the value of the constituent quark masses become small. After searching for the parameters to reproduce good constituent quark masses, we arrive at the optimal numerical values for the parameters $g\Lambda^2=14.63$ and $a=5.12$ giving the constituent quark masses $M=350.38$ MeV, the mixing coefficients $c_{1,\rm gr}=c_{2,\rm gr}=0.684$ and the overlap integral $\det z_{12}=0.069$. In order to get an appropriate value of the constituent quark mass M, it is preferable to use a comparatively large magnitude of the dimensionless volume parameter a. Then in the present paper we have chosen $g\Lambda^2=14.63$ and $a=5.12$. Using the relation $L^3=6\pi^2a/\Lambda^3$ we can see that the value $a=5.12$ corresponds to a ''confinement volume'' of a cube with sides $L=2.10$ fm long. We give in Fig. 2 the Res ground-state NJL energy map for the values of the parameters $g\Lambda^2=14.63$ and $a=5.12$.

In this case, we find only one extreme minimum point of the Res ground-state energy at $x_1=x_2$, i.e., $M_1=M_2$.

In a strict sense, generally it is very difficult to calculate the Res-mean-field excited-state energy self-consistently by a direct-orbital-optimization algorithm. However, we can easily calculate the approximate Res-mean-field excited-state energy $E_{\mathrm{ex}}^{\mathrm{Res}}$, which is given by another solution of the Res-mean-field CI equation called a *resonon*, different from the Res-mean-field ground-state energy $E_{\mathrm{gr}}^{\mathrm{Res}}$. But it is evaluated by using the value of the Res-mean-field variational parameter already determined in the Res-mean-field ground state. The energy difference $E_{\mathrm{ex}}^{\mathrm{Res}}-E_{\mathrm{gr}}^{\mathrm{Res}}$ corresponds to the excitation energy for the Res-excited state above the Res-ground state.

The stability of the vacuum ensured by the Res-mean-field theoretical prescription is intimately connected with the possible occurrence of stable (undamped) excitations of the chirally deformed vacuum. The pionic collective mode is well described as a bound state of quark-antiquark excitations of the chirally deformed vacuum of the original NJL model [9]. Then the energy difference $E_{\mathrm{ex}}^{\mathrm{Res}}-E_{\mathrm{gr}}^{\mathrm{Res}}$ for case I

$$E_{\mathrm{excitation}}^{\mathrm{Res}}=E_{\mathrm{ex}}^{\mathrm{Res}}-E_{\mathrm{gr}}^{\mathrm{Res}} =\frac{2\det z_{12}}{1-(\det z_{12})^2}(H[W]-H[W_{12}]) \quad (\text{for case I}), \tag{5.1}$$

can be interpreted as the pion mass spectrum in the spirit of the Res-mean-field theory. It must be emphasized that we make no use of the concept of the RPA excitation to describe the pion mass spectrum and associated physical quantities, in contrast to the previous works [9–12]. Using the above calculated value, we also can obtain a very good pion mass spectrum $m_\pi=139.70\,\mathrm{MeV}$. Thus we have reproduced the experimental value of the pion mass spectrum $m_\pi=139.6\,\mathrm{MeV}$ in good accuracy. Further it becomes clear that if we adopt a comparatively small magnitude of the dimensionless volume parameter a, a smaller value of the constituent quark masses M and a larger value of the coupling constant g are produced as the result of the present Res-mean-field numerical calculations.

We are now in a position to solve the resonating mean-field equation for *unequal* constituent quark masses. In this case we must search for the energy minimum in the two directions of the quadratic steepest descent Δx_1 and Δx_2 which becomes more complicated than for *equal* constituent quark masses. Let us introduce variational quantities

$$\delta_1 E_{\mathrm{gr}}^{\mathrm{Res}}(x_1,x_2)=\frac{\partial}{\partial x_1}E_{\mathrm{gr}}^{\mathrm{Res}}, \quad \delta_2 E_{\mathrm{gr}}^{\mathrm{Res}}(x_1,x_2)=\frac{\partial}{\partial x_2}E_{\mathrm{gr}}^{\mathrm{Res}}. \tag{5.2}$$

Our tractable-optimization algorithm consists of the following procedure: Let us prepare trial values of x_1 and x_2 suitable for initial values. First, we calculate the overlap integral and the Hamiltonian-matrix elements. Then, from Eqs. (4.16), (4.17), (4.18), and (4.19) we can determine the Res-mean-field ground-state energy and the corresponding mixing coefficients. Next we calculate the quadratic steepest descent $\Delta x_{1,n}$ and $\Delta x_{2,n}$ in the nth iteration step

$$\Delta x_{1,n}=-\frac{1}{\det \delta E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n})}\det\begin{bmatrix} \delta_1 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) & \frac{\partial}{\partial x_2}\delta_1 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) \\ \delta_2 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) & \frac{\partial}{\partial x_2}\delta_2 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) \end{bmatrix}, \tag{5.3}$$

$$\Delta x_{2,n}=-\frac{1}{\det \delta E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n})}\det\begin{bmatrix} \frac{\partial}{\partial x_1}\delta_1 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) & \delta_1 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) \\ \frac{\partial}{\partial x_1}\delta_2 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) & \delta_2 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) \end{bmatrix}, \tag{5.4}$$

where

$$\det \delta E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n})\equiv\det\begin{bmatrix} \frac{\partial}{\partial x_1}\delta_1 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) & \frac{\partial}{\partial x_2}\delta_1 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) \\ \frac{\partial}{\partial x_1}\delta_2 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) & \frac{\partial}{\partial x_2}\delta_2 E_{\mathrm{gr}}^{\mathrm{Res}}(x_{1,n},x_{2,n}) \end{bmatrix}. \tag{5.5}$$

Here $(\partial/\partial x_1)\delta_1 E_{\rm gr}^{\rm Res}(x_{1,n},x_{2,n})$ stands for $(\partial/\partial x_1)\delta_1 E_{\rm gr}^{\rm Res}(x_1,x_2)|_{x_1=x_{1,n},x_2=x_{2,n}}$, etc. We employ the calculated $x_{1,n+1}=x_{1,n}+\Delta x_{1,n}$ and $x_{2,n+1}=x_{2,n}+\Delta x_{2,n}$ as the new trial values of x_1 and x_2 in the next $n+1$th iteration step. We must also continue our Res-mean-field calculations by iterating in succession many time steps until a convergence is achieved.

Our numerical calculations are carried out at the region $g\Lambda^2=12.00$–16.00 and $a=5.00$–9.00. On the contrary to the case of *equal* constituent quark masses, in the present case of *unequal* constituent quark masses we can find in this way a very interesting and good numerical result for the parameters $g\Lambda^2=13.80$ and $a=7.50$ which gives the constituent quark masses $M_1=335.90$ MeV and $M_2=235.82$ MeV, the mixing coefficients $c_{1,\rm gr}=0.810$ and $c_{2,\rm gr}=0.538$ and the overlap integral $\det z_{12}=0.063$. The value $a=7.50$ corresponds to the ''confinement volume'' of a cube with sides $L=2.39$ fm long.

Using these calculated values, from the excitation energy $E_{\rm excitation}^{\rm Res}=E_{\rm ex}^{\rm Res}-E_{\rm gr}^{\rm Res}$ in Eq. (4.16) we can also obtain the very good pion mass spectrum $m_\pi=139.61$ MeV, in excellent agreement with the experimental value of the pion mass spectrum $m_\pi=139.6$ MeV. Introduction of the confinement volume will lead automatically to a nonvanishing pion mass. We assume that the pion mass is exclusively due to this effect. This assumption is in contrast with the traditional idea that the nonvanishing pion mass is due to a nonvanishing current quark mass which causes an explicit chiral symmetry breaking.

We give in Fig. 3 the Res ground-state energy map of NJL for the values of the parameters $g\Lambda^2=13.80$ and $a=7.50$. In this case, contrary to Fig. 2 we can find a drastic structural change in the energy map. Two extreme minimum points of the Res ground-state energy at $x_1=x_2$ and $x_1\neq x_2$ ($M_1\neq M_2$) can be observed in the region $x_1\geqslant x_2$ except at a trivial extreme minimum point $x_1\neq 0$, $x_2=0$. Of course, we are interested in the solution with $x_1\neq x_2$.

VI. ORDER PARAMETER AND PION DECAY CONSTANT

First we consider the solution for *equal* constituent quark masses. In Fig. 1 we observe the behavior of the dimensionless quantity $g\Lambda^2$ which satisfies the ''gap equation'' for case I (3.24). This solution causes the breaking of chiral symmetry because the constituent quark mass is different from zero. Then, the system undergoes a phase transition into a state of broken chiral symmetry. When the constituent quark mass M takes a nonzero value, the S-det $|\Phi(g)\rangle$ $(=|g\rangle)$ is no longer an eigenstate of chirality. Using the Res-mean-field ground-state wave function $|\Psi_{\rm gr}^{\rm Res}\rangle=c_{1,\rm gr}|u_1\rangle+c_{2,\rm gr}|u_2\rangle$, the order parameter for the quarks, which measures the chiral deformation in the Res-mean-field approximation, is given by the expectation value

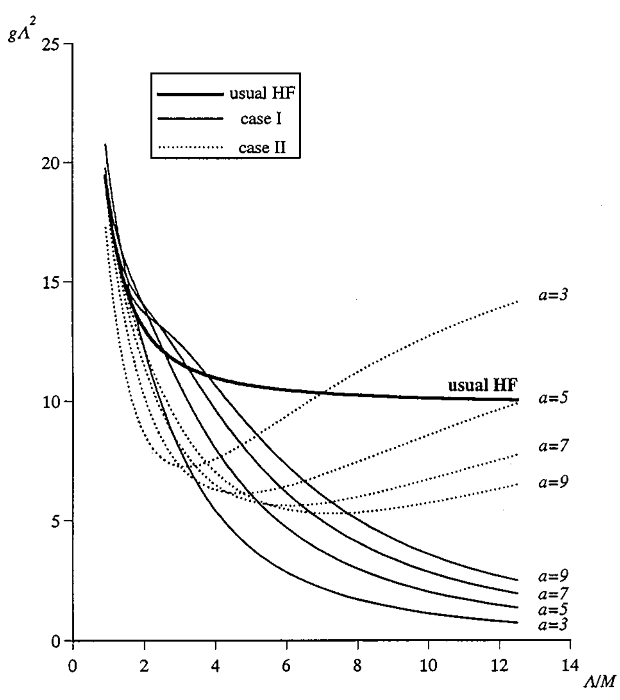

FIG. 1. Λ/M dependence of the dimensionless quantity $g\Lambda^2$ with different dimensionless volume parameters a. Solid and dashed curves represent results for case I and case II, respectively. A thick solid curve represents a result for the usual HF approach.

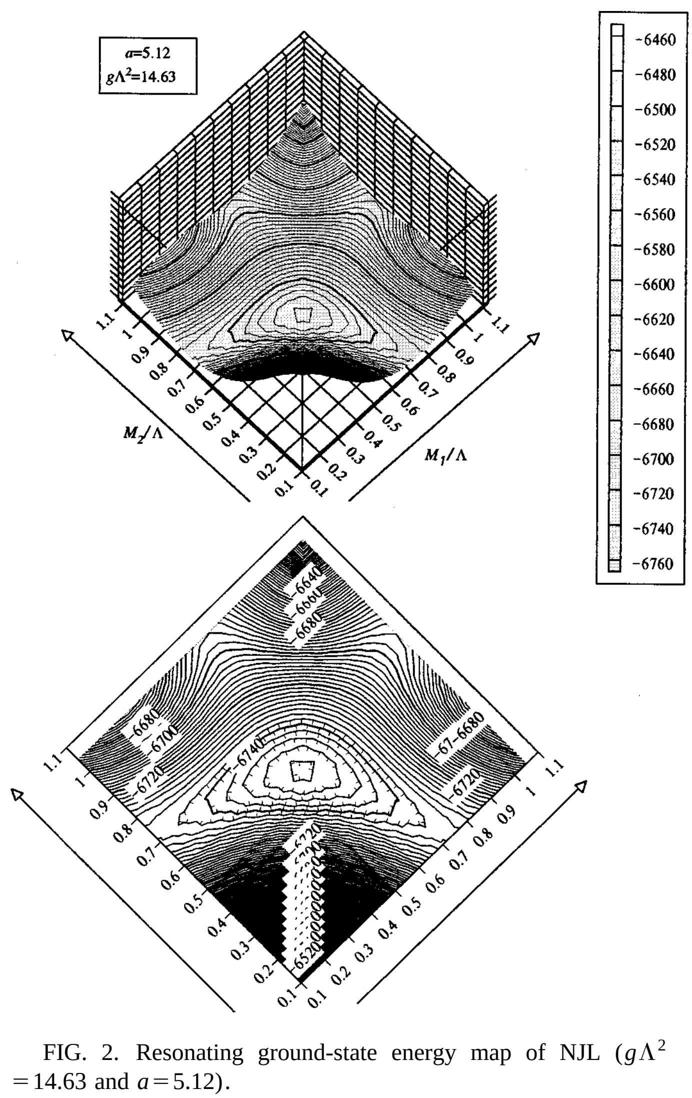

FIG. 2. Resonating ground-state energy map of NJL ($g\Lambda^2=14.63$ and $a=5.12$).

$$\langle\overline{\psi}\psi\rangle=\langle\Psi_{\rm gr}^{\rm Res}|\overline{\psi}\psi|\Psi_{\rm gr}^{\rm Res}\rangle. \tag{6.1}$$

Unfortunately, we find the expection value $\langle\Psi_{\rm gr}^{\rm Res}|\overline{\psi}\psi|\Psi_{\rm gr}^{\rm Res}\rangle$ vanishes trivially as is seen clearly from the explicit structural forms of the usual mean-field density matrices $W_{11,\mathbf{p}}$, Eq. (3.8), and $W_{22,\mathbf{p}}$, Eq. (3.9), for the negative-energy state and the interstate density matrix $W_{12,\mathbf{p}}$, Eq. (3.10), and from the relation $c_{1,\rm gr}=c_{2,\rm gr}$, Eq. (3.16).

However, if we consider the solution for *unequal* constituent quark masses, the order parameter has a nonzero value given by

$$\langle\overline{\psi}\psi\rangle=\langle\Psi_{\rm gr}^{\rm Res}|\overline{\psi}\psi|\Psi_{\rm gr}^{\rm Res}\rangle=c_{1,\rm gr}^2\sum_{\mathbf{p}}\ {\rm Tr}[\beta W_{11,\mathbf{p}}]+c_{2,\rm gr}^2\sum_{\mathbf{p}}\ {\rm Tr}[\beta W_{22,\mathbf{p}}]+c_{1,\rm gr}c_{2,\rm gr}\sum_{\mathbf{p}}\ ({\rm Tr}[\beta W_{12,\mathbf{p}}]+{\rm Tr}[\beta W_{12,\mathbf{p}}^\dagger])\prod_{\mathbf{p}}\ \det z_{12,\mathbf{p}}\theta(\Lambda^2-p^2), \tag{6.2}$$

from which the quantity per normalization volume $-\{\langle\overline{\psi}\psi\rangle/V\}^{1/3}$ is evaluated as

$$-\{\langle\overline{\psi}\psi\rangle/V\}^{1/3}=\frac{\Lambda}{(2\pi^2)^{1/3}}\left\{c_{1,\rm gr}^2x_1v(x_1)-c_{2,\rm gr}^2x_2v(x_2)+c_{1,\rm gr}c_{2,\rm gr}\det z_{12}\frac{1}{x_1+x_2}\left[\sqrt{1+x_1^2}+\frac{x_1^2}{2}v(x_1)-\sqrt{1+x_2^2}-\frac{x_2^2}{2}v(x_2)\right]\right\}^{1/3}. \tag{6.3}$$

In the above, if we set $x_1=x_2$ and $c_{1,\rm gr}=c_{2,\rm gr}$ the order parameter vanishes trivially. On the other hand, if we assume $c_{1,\rm gr}=1$ and $c_{2,\rm gr}=0$, the above equation just coincides with the formula for the order parameter given in [9]. Substituting the solution for the parameters $g\Lambda^2=13.80$ ($\Lambda=631.0$ MeV) and $a=7.50$ presented in the preceeding section, i.e., $x_1=0.532$, $x_2=0.374$, $c_{1,\rm gr}=0.810$, $c_{2,\rm gr}=0.538$, and $\det z_{12}=0.063$ into Eq. (6.3), we are led to a numerical result $-\{\langle\overline{\psi}\psi\rangle/V\}^{1/3}=129.80$ MeV. This value is a little bit small when compared with the theoretical one and the experimental one given in Refs. [10] and [12]. However, if the degrees of freedom of isospin, flavor, and color are fully taken into consideration, it may be expected that a much improved value for $-\{\langle\overline{\psi}\psi\rangle/V\}^{1/3}$ will be obtained.

Thus, by taking into account quantum- and dynamical-tunneling effects between the two S-dets with *unequal* constituent quark masses and with different correlation structures, the present Res-mean-field approach throws some new light on the dynamics of chiral-symmetry breaking and of the collective pionic state.

The Res-mean-field method is able to describe an associated decay process if we notice the similarity of the forms of the interstate density matrix and the generator which produces the RPA pionic state given in [9].

In the usual RPA, the pion decay constant f_π is defined as the time component of the axial-vector matrix element $\langle 0|j_5|\pi_{\mathbf{p}}\rangle=f_\pi[\omega(\mathbf{p})]^{1/2}$ [$\omega(\mathbf{p})$ being a pion mass spectrum], $j_5=\Sigma_{j=1}^N\gamma_j^5e^{-i\mathbf{p}\cdot\mathbf{r}_j}$ for the RPA pionic state $|\pi_{\mathbf{p}}\rangle$ of momentum $\mathbf{p}$ and vacuum $|0\rangle$ [9]. In the Res-mean-field RPA [18] the pion decay constant f_π may be described as $\langle 0^{\rm Res}|j_5|\pi_{\mathbf{p}}^{\rm Res}\rangle=f_\pi[E_{\rm excitation}^{\rm Res}]^{1/2}$ for the Res-mean-field RPA pionic state $|\pi_{\mathbf{p}}^{\rm Res}\rangle$ of momentum $\mathbf{p}$ and vacuum $|0^{\rm Res}\rangle$. Both in the usual RPA and in the Res-mean-field RPA an operator similar in form to that of the interstate density matrix $W_{12,\mathbf{p}}$ plays a crucial role as is shown in Refs. [10, 12], and [19], respectively. The Res-mean-field RPA pionic state can be approximated as $|\pi_{\mathbf{p}}^{\rm Res}\rangle\simeq\mathcal{N}W_{12,\mathbf{p}}^\dagger|0^{\rm Res}\rangle$, where $\mathcal{N}$ is the normalization factor to be determined later. Then, within the framework of the Res-mean-field approximation, by using the Res-mean-field excited-state wave function $|\Psi_{\rm ex}^{\rm Res}\rangle=c_{1,\rm ex}|u_1\rangle+c_{2,\rm ex}|u_2\rangle$ and the helicity operator $S_{\mathbf{p}}$ defined as $S_{\mathbf{p}}=\Sigma\cdot\mathbf{p}/|\mathbf{p}|$ we get

$$f_\pi=\langle 0^{\rm Res}|j_5|\pi_{\mathbf{p}}^{\rm Res}\rangle[E_{\rm excitation}^{\rm Res}]^{-1/2}\simeq\mathcal{N}\langle 0^{\rm Res}|j_5W_{12,\mathbf{p}}^\dagger|0^{\rm Res}\rangle[E_{\rm excitation}^{\rm Res}]^{-1/2}\simeq\mathcal{N}\langle\Psi_{\rm gr}^{\rm Res}|\Sigma_{i=1}^N(\gamma_i^5S_{\mathbf{p}_i})|\Psi_{\rm ex}^{\rm Res}\rangle[E_{\rm excitation}^{\rm Res}]^{-1/2}$$
$$\Rightarrow\mathcal{N}\left\{c_{1,\rm gr}c_{1,\rm ex}\sum_{\mathbf{p}}\ {\rm Tr}[(\gamma^5S_{\mathbf{p}})W_{11,\mathbf{p}}]+c_{2,\rm gr}c_{2,\rm ex}\sum_{\mathbf{p}}\ {\rm Tr}[(\gamma^5S_{\mathbf{p}})W_{22,\mathbf{p}}]+\left(c_{1,\rm gr}c_{2,\rm ex}\sum_{\mathbf{p}}\ {\rm Tr}[(\gamma^5S_{\mathbf{p}})]W_{12,\mathbf{p}}+c_{2,\rm gr}c_{1,\rm ex}\sum_{\mathbf{p}}\ {\rm Tr}[(\gamma^5S_{\mathbf{p}})W_{12,\mathbf{p}}^\dagger]\right)\prod_{\mathbf{p}}\ \det z_{12,\mathbf{p}}\theta(\Lambda^2-p^2)\right\}[E_{\rm excitation}^{\rm Res}]^{-1/2}. \tag{6.4}$$

Here we have used a slightly modified definition of the matrix element of γ^5 to get a significant nonzero value of the f_π. The mixing coefficients $c_{1,\rm ex}$ and $c_{2,\rm ex}$ are determined through Eqs. (4.18) and (4.19) and the orthogonality condition $\langle\Psi_{\rm gr}^{\rm Res}|\Psi_{\rm ex}^{\rm Res}\rangle=0$.

Let us consider again the solution for *equal* constituent quark mass as an elementary exercise. We also find the matrix element $\langle\Psi_{\rm gr}^{\rm Res}|\Sigma_{i=1}^N(\gamma_i^5S_{\mathbf{p}_i})|\Psi_{\rm ex}^{\rm Res}\rangle$ vanishes trivially as is seen clearly from the explicit forms of $W_{11,\mathbf{p}}$, Eq. (3.8), $W_{22,\mathbf{p}}$, Eq. (3.9), and $W_{12,\mathbf{p}}$, Eq. (3.10) and from the relations $c_{2,\rm gr}=c_{1,\rm gr}$ and $c_{2,\rm ex}=-c_{1,\rm ex}$, Eq. (3.16).

However, if we consider the solution for *unequal* constituent quark masses, the matrix element $\langle\Psi_{\rm gr}^{\rm Res}|\Sigma_{i=1}^N(\gamma_i^5S_{\mathbf{p}_i})|\Psi_{\rm ex}^{\rm Res}\rangle$ obtains a nonzero value. First we must evaluate the normalization factor. For the Res-mean-field RPA pionic state $|\pi_{\mathbf{p}}^{\mathrm{Res}}\rangle = \mathcal{N} W_{12,\mathbf{p}}^{\dagger}|0^{\mathrm{Res}}\rangle$, the normalization factor follows from the normalization requirement

$$\sum_{\mathbf{p}} \langle \pi_{\mathbf{p}}^{\mathrm{Res}}|\pi_{\mathbf{p}}^{\mathrm{Res}}\rangle = 1 = \mathcal{N}^2 \langle 0^{\mathrm{Res}}|\sum_{\mathbf{p}} W_{12,\mathbf{p}} W_{12,\mathbf{p}}^{\dagger}|0^{\mathrm{Res}}\rangle$$
$$= \mathcal{N}^2 \langle 0^{\mathrm{Res}}|\sum_{\mathbf{p}} [W_{12,\mathbf{p}}, W_{12,\mathbf{p}}^{\dagger}]|0^{\mathrm{Res}}\rangle, \tag{6.5}$$

which is approximated as

$$1 \simeq \mathcal{N}^2 \langle \Psi_{\mathrm{gr}}^{\mathrm{Res}}|\sum_{\mathbf{p}} [W_{12,\mathbf{p}}, W_{12,\mathbf{p}}^{\dagger}] \det z_{12,\mathbf{p}}|\Psi_{\mathrm{gr}}^{\mathrm{Res}}\rangle. \tag{6.6}$$

For the sake of simplicity, instead of Eq. (6.6), we use an approximate normalization

$$1 \simeq \mathcal{N}^2 \Bigg[\langle \Psi_{\mathrm{gr}}^{\mathrm{Res}}|\sum_{\mathbf{p}} \theta(\Lambda^2 - p^2) \sum_{\mathbf{p}} \times \mathrm{Tr}\{[W_{12,\mathbf{p}}, W_{12,\mathbf{p}}^{\dagger}]\}^2 \left(\frac{\det z_{12,\mathbf{p}}}{\mathrm{Tr}[I_4]} \right)^2 |\Psi_{\mathrm{gr}}^{\mathrm{Res}}\rangle \Bigg]^{1/2}, \tag{6.7}$$

from which we obtain

$$\mathcal{N} = \Bigg[\langle \Psi_{\mathrm{gr}}^{\mathrm{Res}}|\sum_{\mathbf{p}} \theta(\Lambda^2 - p^2) \sum_{\mathbf{p}} \times \mathrm{Tr}\{[W_{12,\mathbf{p}}, W_{12,\mathbf{p}}^{\dagger}]\}^2 \left(\frac{\det z_{12,\mathbf{p}}}{\mathrm{Tr}[I_4]} \right)^2 |\Psi_{\mathrm{gr}}^{\mathrm{Res}}\rangle \Bigg]^{-1/4}. \tag{6.8}$$

On the other hand, from the explicit expression for the inter-state density matrix $W_{12,\mathbf{p}}$, Eq. (4.11), we derive easily a commutation relation

$$[W_{12,\mathbf{p}}, W_{12,\mathbf{p}}^{\dagger}] = \frac{E_{1\mathbf{p}} E_{2\mathbf{p}} - \mathbf{p}^2 + M_1 M_2}{(M_1 + M_2)^2 \mathbf{p}^2} [-(E_{1\mathbf{p}} - E_{2\mathbf{p}}) \gamma^5 \mathbf{\Sigma} \cdot \mathbf{p} + (E_{1\mathbf{p}} M_2 + E_{2\mathbf{p}} M_1) \beta] \theta(\Lambda^2 - p^2). \tag{6.9}$$

With the use of the relation $\det z_{12,\mathbf{p}} = -1/2[1 + (\mathbf{p}^2 - M_1 M_2)/(E_{1\mathbf{p}} E_{2\mathbf{p}})]$, Eq. (4.4), and the above commutation relation, we get a matrix-valued identity relation

$$\{[W_{12,\mathbf{p}}, W_{12,\mathbf{p}}^{\dagger}]\}^2 (\det z_{12,\mathbf{p}})^2 = \frac{1}{2} \left[1 - \frac{\mathbf{p}^2}{E_{1\mathbf{p}} E_{2\mathbf{p}}} + \beta_{1\mathbf{p}} \beta_{2\mathbf{p}} \right] I_4 \theta(\Lambda^2 - p^2). \tag{6.10}$$

Substitution of Eq. (6.10) into Eq. (6.8) leads to an explicit expression for the normalization factor $\mathcal{N}$

$$\mathcal{N} = 2 \left\{ \int \frac{d^3\mathbf{p}}{(2\pi)^3} \theta(\Lambda^2 - p^2) \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{1}{2} \left[1 - \frac{\mathbf{p}^2}{E_{1\mathbf{p}} E_{2\mathbf{p}}} + \beta_{1\mathbf{p}} \beta_{2\mathbf{p}} \right] 4 \theta(\Lambda^2 - p^2) \right\}^{-1/4}$$
$$= 2 \Bigg\{ V \frac{1}{6\pi^2} \Lambda^3 V \frac{1}{3\pi^2} \Lambda^3 \Bigg[1 - (1 - 2x_1^2 - 3x_1 x_2 - x_2^2) \sqrt{\frac{1 + x_1^2}{1 + x_2^2}} - x_1 (2x_1^2 + 3x_1 x_2 + 2x_2^2) E\left(\tan^{-1} \frac{1}{x_2}, \sqrt{1 - \frac{x_2^2}{x_1^2}} \right)$$
$$+ x_1 x_2^2 F\left(\tan^{-1} \frac{1}{x_2}, \sqrt{1 - \frac{x_2^2}{x_1^2}} \right) \Bigg] \Bigg\}^{-1/4} \quad (x_1 \geqslant x_2). \tag{6.11}$$

By using the explicit forms of $W_{11,\mathbf{p}}$, Eq. (4.9), $W_{22,\mathbf{p}}$, Eq. (4.10), and $W_{12,\mathbf{p}}$, Eq. (4.11), the matrix element $\langle \Psi_{\mathrm{gr}}^{\mathrm{Res}}|\Sigma_{i=1}^{N} (\gamma_i^5 S_{\mathbf{p}_i})|\Psi_{\mathrm{ex}}^{\mathrm{Res}}\rangle$ is calculated as

$$\langle \Psi_{\mathrm{gr}}^{\mathrm{Res}}|\Sigma_{i=1}^{N} (\gamma_i^5 S_{\mathbf{p}_i})|\Psi_{\mathrm{ex}}^{\mathrm{Res}}\rangle = -V \frac{1}{3\pi^2} \Lambda^3 \Big\{ c_{1,\mathrm{gr}} c_{1,\mathrm{ex}} [\sqrt{1 + x_1^2}(1 - 2x_1^2) + 2x_1^3] + c_{2,\mathrm{gr}} c_{2,\mathrm{ex}} [\sqrt{1 + x_2^2}(1 - 2x_2^2) + 2x_2^3]$$
$$+ (c_{1,\mathrm{gr}} c_{2,\mathrm{ex}} + c_{2,\mathrm{gr}} c_{1,\mathrm{ex}}) \cdot \det z_{12} \frac{1}{x_1 + x_2} [x_1 (1 + x_2^2)^{3/2} + x_2 (1 + x_1^2)^{3/2} - x_1 x_2 (x_1^2 + x_2^2)] \Big\}. \tag{6.12}$$

Then finally we obtain the ratio of the pion decay constant f_π to the square root of the normalization volume $\sqrt{V}$

$$\frac{f_\pi}{\sqrt{V}} = -\frac{4\Lambda}{\sqrt{6\sqrt{2}}\pi}\left[\frac{E^{\mathrm{Res}}_{\mathrm{excitation}}}{\Lambda}\right]^{-1/2}\Bigg[1-(1-2x_1^2-3x_1x_2-x_2^2)\sqrt{\frac{1+x_1^2}{1+x_2^2}}-x_1(2x_1^2+3x_1x_2+2x_2^2)E\left(\tan^{-1}\frac{1}{x_2},\sqrt{1-\frac{x_2^2}{x_1^2}}\right)$$
$$+x_1x_2^2F\left(\tan^{-1}\frac{1}{x_2},\sqrt{1-\frac{x_2^2}{x_1^2}}\right)\Bigg]^{-1/4}\Bigg\{c_{1,\mathrm{gr}}c_{1,\mathrm{ex}}[\sqrt{1+x_1^2}(1-2x_1^2)+2x_1^3]+c_{2,\mathrm{gr}}c_{2,\mathrm{ex}}[\sqrt{1+x_2^2}(1-2x_2^2)+2x_2^3]$$
$$+(c_{1,\mathrm{gr}}c_{2,\mathrm{ex}}+c_{2,\mathrm{gr}}c_{1,\mathrm{ex}})\cdot\det z_{12}\frac{1}{x_1+x_2}[x_1(1+x_2^2)^{3/2}+x_2(1+x_1^2)^{3/2}-x_1x_2(x_1^2+x_2^2)]\Bigg\}\quad (x_1\geqslant x_2). \tag{6.13}$$

Substituting the solution for the parameters $g\Lambda^2=13.80$ ($\Lambda=631.0\,\mathrm{MeV}$) and $a=7.50$ in the preceding section, i.e., $x_1=0.532$, $x_2=0.374$, $c_{1,\mathrm{gr}}=0.810$, $c_{2,\mathrm{gr}}=0.538$, $c_{1,\mathrm{ex}}=0.590$, $c_{2,\mathrm{ex}}=-0.845$, and $\det z_{12}=0.063$ into Eq. (6.13), we are led to a numerical result $f_\pi/\sqrt{V}=29.7\,\mathrm{MeV}$. This value is a little bit small when compared with the theoretical one and the experimental one given in Refs. [10] and [12]. However, if the degrees of freedom of the isospin, the flavor, and the color are taken into consideration fully, it may be expected to get a much improved value for the $f_\pi/\sqrt{V}$. The normalization factor is also computed as $\mathcal{N}=0.0009$ whose value is too small but plays a crucial role in achieving a reasonable value of the $f_\pi/\sqrt{V}$.

VII. SUMMARY AND CONCLUDING REMARKS

We will now describe in detail other numerical quantities in the Res-mean-field approach to the NJL model. In the Res-mean-field approximation the overlap integral $\det z_{12}$ between the two S-dets as well as the interstate density matrix W_{12} plays an important role, allowing to take into account a quantum tunneling effect between the two S-dets. To get a finite value of the $\det z_{12}$ it is necessary to introduce the dimensionless parameter a which gives the ‘‘confinement volume.’’

Under the use of the S-dets with *equal* constituent quark masses, the overlap integral $\det z_{12}$ is plotted as a function of M/Λ for the different dimensionless parameters a (see Fig. 4). The value of the $\det z_{12}$ decreases rapidly as the constituent quark mass becomes heavier and as the confinement volume is increased. This result is considered to be reasonable.

Under the use of the S-dets with *unequal* constituent quark masses, the overlap integral $\det z_{12}$ is also plotted as a function of M_1/Λ and M_2/Λ for the two sets of parameters $a=5.12$, $g\Lambda^2=14.63$ and $a=7.50$, $g\Lambda^2=13.80$ (see Fig. 5). These sets of parameters give the directly optimized solutions of the Res-mean-field equations for the *equal* constituent quark masses and for the *unequal* constituent quark masses, respectively. The value of the $\det z_{12}$ for the former set shows a more gradual decrease than that for the latter set as both the constituent quark masses become heavier. The latter $a=7.50$ corresponds to the confinement volume of a cube with sides $L=2.38\,\mathrm{fm}$ long.

To show the advantage of the Res-mean-field theory for a fermion system with large quantum fluctuations over the usual mean-field theory, in this paper we have applied it to the naive NJL model without isospin. For the sake of simplicity, a state with large quantum fluctuations is approximated by the superposition of two Dirac seas, the nonorthogonal two S-dets with different correlation structures. We have treated two cases: in the first case the Dirac seas are composed of *equal* constituent quark masses, while in the second the quark masses are *unequal*. We have made a direct optimization of the Res-mean-field orbitals by variations of the Res-mean-field ground-state energy with respect to the Res-mean-field parameters, constituent quark masses. The Res-mean-field ground and excited states generated with the two S-dets explain most of the pion mass spectrum.

We also have investigated, in the framework of the NJL

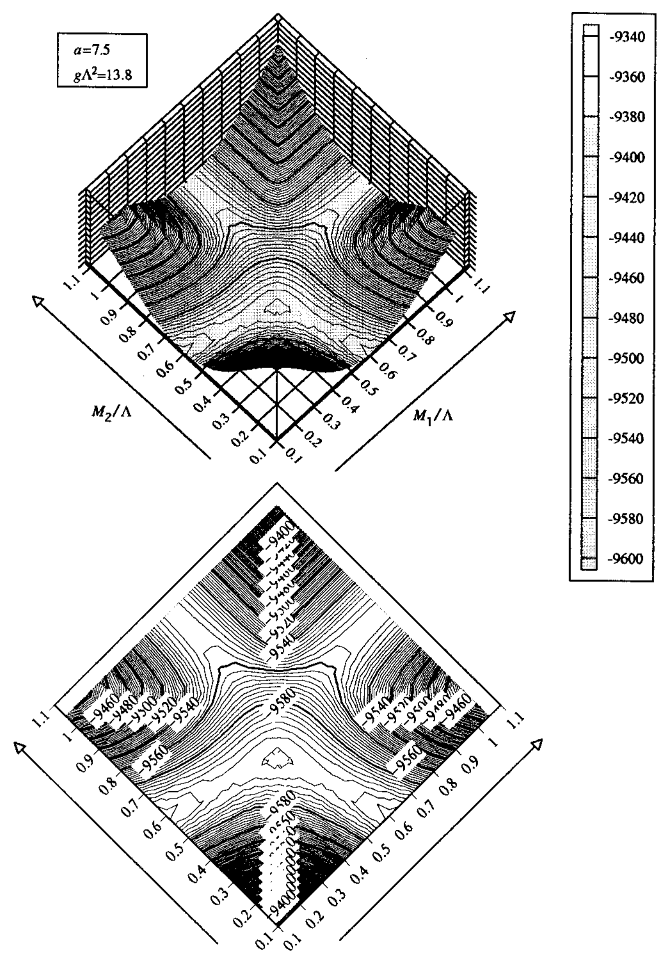

FIG. 3. Resonating ground-state energy map of NJL ($g\Lambda^2=13.80$ and $a=7.50$).

TABLE I. Use of the S-dets with *equal* constituent quark masses. Pionic properties in the context of the Res-mean-field theory with *equal* constituent quark masses. The asterisk denotes results concerning the NJL in the harmonic order, taken from [10]. We also include in brakets some experimental or phenomenological values. The Res-MFT means the resonating mean-field theory. The output value 12.0 of $g\Lambda^2$ in the column TDHF corresponds to the output value 2.0 of the same quantity in [10] if we take the degree of the freedom of the flavor $N_f=2$ and that of the color $N_c=3$.

		NJL model	
		Res-MFT	TDHF
Inputs	a	5.12	
	Λ (MeV)	631.0	631.0*
Outputs	$g\Lambda^2$	14.63	12.0
	M (MeV)	350.38	335.0* (350)
	$-\langle\bar{\psi}\psi\rangle^{1/3}$ (MeV)	0	246.6* (225±25)
	m_π (MeV)	139.70	138.0* (139.6)
	f_π (MeV)	0	93.0* (93)

TABLE II. Use of the S-dets with *unequal* constituent quark masses. Pionic properties in the context of the Res-mean-field theory with *unequal* constituent quark masses.

		NJL model	
		Res-MFT	TDHF
Inputs	a	7.50	
	Λ (MeV)	631.0	631.0*
Outputs	$g\Lambda^2$	13.80	12.0
	M_1, M_2 (MeV)	335.90, 235.82	335.0* (350)
	$-\langle\bar{\psi}\psi\rangle^{1/3}$ (MeV)	129.80	246.6* (225±25)
	m_π (MeV)	139.61	138.0* (139.6)
	f_π (MeV)	29.70	93.0* (93)

model, effects of the explicit chiral-symmetry breaking on the associated properties of the Dirac sea and the collective pionic state in the sprit of the Res-mean-field approximation.

The present treatment has following characteristic points quite similar to those in [9]: (i) There are actually three model parameters Λ (the cutoff parameter), g (the coupling constant), and a (the dimensionless volume parameter). (ii) The coupling constant g does not enter the vacuum properties as is seen from the explicit form of the S-det $|\Phi(g)\rangle$ $(=|g\rangle)$, Eq. (3.1). (iii) The regime of the results depends only on the dimensionless ratio M_1/Λ and M_2/Λ and only the constituent quark masses M_1 and M_2 determine the energy (or length) scale through Eq. (4.20). We interpret M_1 and M_2 $(M_1 \geqslant M_2)$ as the constituent quark masses and use as the variational parameters. But only the heavier one has a significant physical meaning because the magnitude of square of the corresponding mixing coefficient $c^2_{1,\mathrm{gr}}$ is much larger than that of the other, $c^2_{2,\mathrm{gr}}$.

Finally, summarizing, we present in Tables I and II numerical results for various physical quantities. Especially, the numerical values of $g\Lambda^2$, constituent quark masses M_1, M_2, pion mass m_π, order parameter $-\{\langle\bar{\psi}\psi\rangle/V\}^{1/3}$ and pion decay constant $f_\pi/\sqrt{V}$ tabulated in Table II compare comparatively well with the experimental datas.

The radical spirit of the Res-mean-field theory may be expected to open a new field for the exploration of the low-energy hadron physics using the strong analogy between a chiral effective Hamiltonian with four-fermion interaction and a familiar nonrelativistic fermion two-body Hamiltonian. The present calculation is oversimplified as far as we consider only the two S-dets. Then the following problems remain open questions: (1) The consideration of the degrees of freedom of the isospin, the flavor, and the color. (2) The inclusion of collective σ mesonic state. (3) Chiral projection to project out good chiral state if small current quark masses are introduced.

Very recently, one of the present authors (J. da P.) and his collaborators investigated the connection between the linear σ model and the NJL model on the basis of the usual mean-field theory. They have shown the conditions for soliton formation and the stability of the soliton when the Dirac sea is included [20]. Then we have another interesting problem to

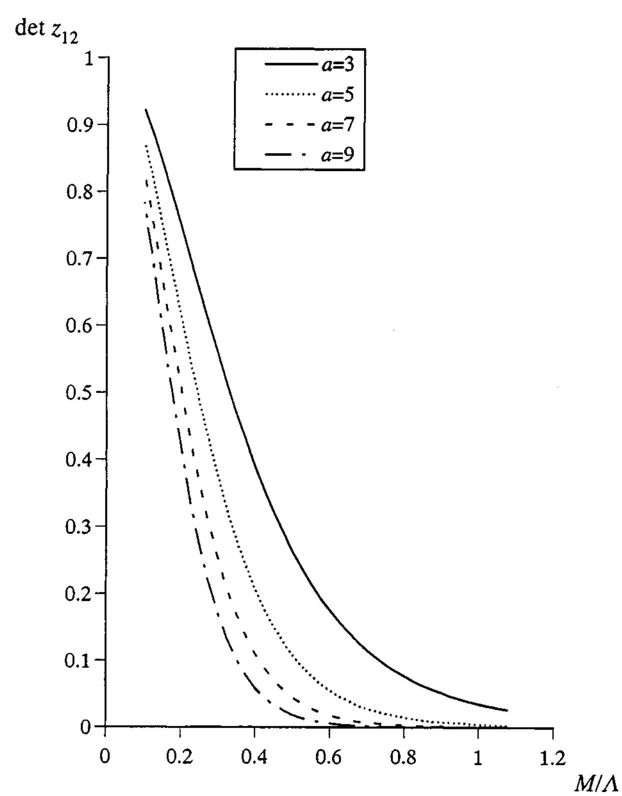

FIG. 4. Overlap integral $\det z_{12}$ as a function of M/Λ for the different parameters a.

be solved in the near future: (4) The relation between the σ model with quarks and the present Res-mean-field theoretical approach to the NJL model.

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APPENDIX A: MATRIX ELEMENT OF THE HAMILTONIAN WITH EQUAL CONSTITUENT QUARK MASSES

Here we give detailed computation of the matrix element of the Hamiltonian (2.1) $\langle u_1|H|u_2\rangle$ along the same way as the one in [9]. Using the explicit expression for the interstate density matrix $W_{12,\mathbf{p}}$, Eq. (3.10), for the kinetic part we have

$$\mathrm{Tr}[\gamma^5\mathbf{\Sigma}\cdot\mathbf{p}W_{12,\mathbf{p}}]=-2E_{\mathbf{p}}\theta(\Lambda^2-p^2). \tag{A1}$$

For the direct term of the interaction part, we have trivial relations

$$\mathrm{Tr}[\beta W_{12,\mathbf{p}}]=0, \quad \mathrm{Tr}[\beta\gamma^5 W_{12,\mathbf{p}}]=0. \tag{A2}$$

For the exchange terms of the interaction part, we have

$$\mathrm{Tr}[\beta(1)W_{12,\mathbf{p}_1}(1)\beta(2)W_{12,\mathbf{p}_2}(2)] =\left[1-\frac{\mathbf{p}_1\cdot\mathbf{p}_2}{\mathbf{p}_1^2\mathbf{p}_2^2}(E_{\mathbf{p}_1}E_{\mathbf{p}_2}-M^2)\right]\theta(\Lambda^2-p^2), \tag{A3}$$

$$\mathrm{Tr}[\beta(1)\gamma^5(1)W_{12,\mathbf{p}_1}(1)\beta(2)\gamma^5(2)W_{12,\mathbf{p}_2}(2)] =\left[-1+\frac{\mathbf{p}_1\cdot\mathbf{p}_2}{\mathbf{p}_1^2\mathbf{p}_2^2}(E_{\mathbf{p}_1}E_{\mathbf{p}_2}+M^2)\right]\theta(\Lambda^2-p^2). \tag{A4}$$

Performing the space integration and both the summation and the product over $\mathbf{p}$, $\mathbf{p}_1$, and $\mathbf{p}_2$, then the matrix element of the Hamiltonian is transformed to

$$\langle u_1|H|u_2\rangle=\int d^3\mathbf{r}\Sigma_{\mathbf{p}}H[W_{12,\mathbf{p}}]\prod_{\mathbf{p}} \det z_{12,\mathbf{p}}\theta(\Lambda^2-p^2) =H[W_{12}]\cdot\det z_{12}. \tag{A5}$$

Changing the summation over $\mathbf{p}$ into the integration over $\mathbf{p}$, $H[W_{12}]$ is given simply as

$$H[W_{12}]=\int d^3\mathbf{r}\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[\gamma^5\mathbf{\Sigma}\cdot\mathbf{p}W_{12,\mathbf{p}}] -2g\int d^3\mathbf{r}\left(\int\frac{d^3\mathbf{p}}{(2\pi)^3}\theta(\Lambda^2-p^2)\right)^2, \tag{A6}$$

which is calculated to be

$$H[W_{12}]=-2\left[\int\frac{d^3\mathbf{p}}{(2\pi)^3}E_p\theta(\Lambda^2-p^2)\right]V -2g\left[\int\frac{d^3\mathbf{p}}{(2\pi)^3}\theta(\Lambda^2-p^2)\right]^2 V. \tag{A7}$$

From Eq. (A7) thus we can reach to a desired form of the matrix element of the Hamiltonian, i.e., Eq. (3.13).

In [9] it has already been proved that $H[W_{11}]$ is invariant under a chiral transformation. And then $H[W_{22}]$ is also invariant. We can easily prove that $H[W_{12}]$ becomes invariant under the chiral transformation as can be seen in detail in Appendix C. As the consequence of this fact, the expectation value of the NJL Hamiltonian (2.1) by the superposed wave function $c_1|u_1\rangle+c_2|u_2\rangle$ becomes invariant under the chiral transformation.

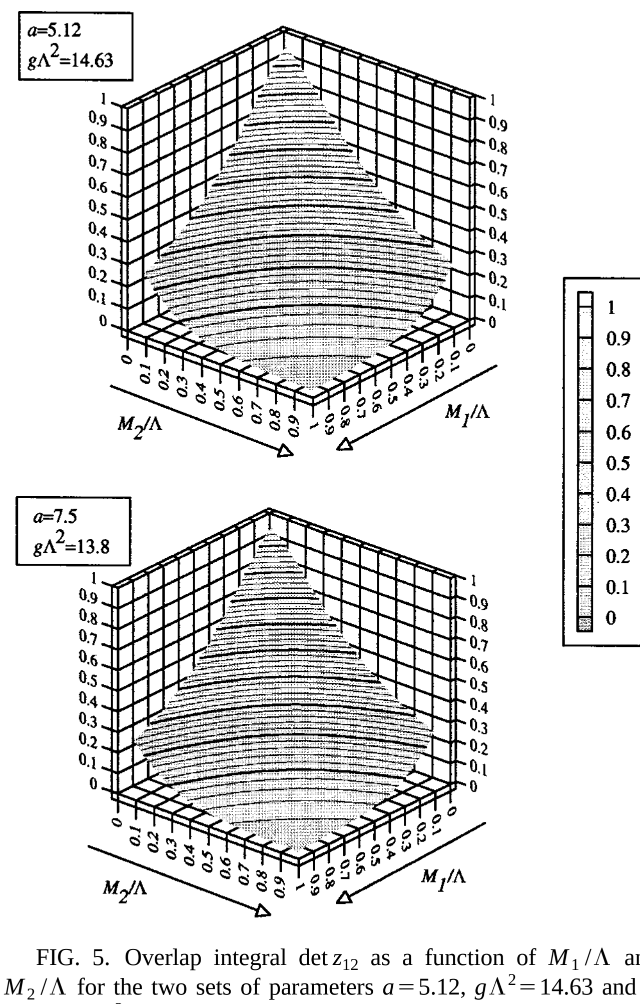

FIG. 5. Overlap integral $\det z_{12}$ as a function of M_1/Λ and M_2/Λ for the two sets of parameters $a=5.12$, $g\Lambda^2=14.63$ and $a=7.50$, $g\Lambda^2=13.80$.

APPENDIX B: CALCULATIONS OF THE OVERLAP INTEGRAL AND ITS PARTIAL DIFFERENTIALS

In this appendix we present some useful formulas of elliptic integrals. These are taken or easily derived from formulas in [17]. First, to calculate the overlap integral $\det z_{12}$, it is convenient to use the following reduction formulas of algebraic integrands to the elliptic functions E and F:

$$\int_0^\Lambda dp\,\frac{p^2}{\sqrt{p^2+M_1^2}\sqrt{p^2+M_2^2}}=\begin{cases}\Lambda\sqrt{\dfrac{1+x_1^2}{1+x_2^2}}-\Lambda x_1 E\left(\tan^{-1}\dfrac{1}{x_2},\sqrt{1-\dfrac{x_2^2}{x_1^2}}\right), & (x_1\geqslant x_2),\\ \Lambda\sqrt{\dfrac{1+x_2^2}{1+x_1^2}}-\Lambda x_2 E\left(\tan^{-1}\dfrac{1}{x_1},\sqrt{1-\dfrac{x_1^2}{x_2^2}}\right), & (x_2\geqslant x_1),\end{cases}\tag{B1}$$

$$\int_0^\Lambda dp\,\frac{p^4}{\sqrt{p^2+M_1^2}\sqrt{p^2+M_2^2}}$$
$$=\begin{cases}\dfrac{1}{3}\Lambda^3(1-2x_1^2-x_2^2)\sqrt{\dfrac{1+x_1^2}{1+x_2^2}}+\dfrac{1}{3}\Lambda^3 x_1\left[2(x_1^2+x_2^2)E\left(\tan^{-1}\dfrac{1}{x_2},\sqrt{1-\dfrac{x_2^2}{x_1^2}}\right)-x_2^2F\left(\tan^{-1}\dfrac{1}{x_2},\sqrt{1-\dfrac{x_2^2}{x_1^2}}\right)\right], & (x_1\geqslant x_2),\\ \dfrac{1}{3}\Lambda^3(1-2x_2^2-x_1^2)\sqrt{\dfrac{1+x_2^2}{1+x_1^2}}+\dfrac{1}{3}\Lambda^3 x_2\left[2(x_2^2+x_1^2)E\left(\tan^{-1}\dfrac{1}{x_1},\sqrt{1-\dfrac{x_1^2}{x_2^2}}\right)-x_1^2F\left(\tan^{-1}\dfrac{1}{x_1},\sqrt{1-\dfrac{x_1^2}{x_2^2}}\right)\right], & (x_2\geqslant x_1).\end{cases}\tag{B2}$$

To calculate partial differentials of the overlap integral $\det z_{12}$, formulas for partial differentiation of the elliptic integrals E and F used in the text are the following, which are also taken from formulas in [17]:

$$\frac{\partial E(\phi,k)}{\partial k}=\frac{E(\phi,k)-F(\phi,k)}{k},\tag{B3}$$

$$\frac{\partial E(\phi,k)}{\partial\phi}=\sqrt{1-k^2\sin^2\phi},\tag{B4}$$

$$\frac{\partial F(\phi,k)}{\partial k}=\frac{E(\phi,k)-k'^2F(\phi,k)}{kk'^2}-\frac{k\sin\phi\cos\phi}{k'^2\sqrt{1-k^2\sin^2\phi}},\quad k'=\sqrt{1-k^2},\tag{B5}$$

$$\frac{\partial F(\phi,k)}{\partial\phi}=\frac{1}{\sqrt{1-k^2\sin^2\phi}}.\tag{B6}$$

Using the above formulas (B3)–(B6), partial differentials of the overlap integral $\det z_{12}$ given by Eqs. (4.7) and (4.8) with respect to the variables x_1 and x_2, respectively, are calculated as

$$\frac{\partial}{\partial x_1}\det z_{12}=a(\det z_{12})\frac{1}{x_1+x_2}\left[1-3x_1x_2-3x_1^2+3x_1^2(x_1+x_2)\tan^{-1}\frac{1}{x_1}-(1-2x_1^2+2x_2^2)\sqrt{\frac{1+x_1^2}{1+x_2^2}}\right.$$
$$\left.-x_1(2x_1^2-x_2^2)E\left(\tan^{-1}\frac{1}{x_2},\sqrt{1-\frac{x_2^2}{x_1^2}}\right)+x_1x_2^2F\left(\tan^{-1}\frac{1}{x_2},\sqrt{1-\frac{x_2^2}{x_1^2}}\right)\right],\quad (x_1\geqslant x_2),\tag{B7}$$

$$\frac{\partial}{\partial x_2}\det z_{12}=a(\det z_{12})\frac{1}{x_2+x_1}\left[1-3x_2x_1-3x_2^2+3x_2^2(x_2+x_1)\tan^{-1}\frac{1}{x_2}-(1-x_2^2+x_1^2)\sqrt{\frac{1+x_1^2}{1+x_2^2}}\right.$$
$$\left.-x_1(2x_2^2-x_1^2)E\left(\tan^{-1}\frac{1}{x_2},\sqrt{1-\frac{x_2^2}{x_1^2}}\right)+x_2^2x_1F\left(\tan^{-1}\frac{1}{x_2},\sqrt{1-\frac{x_2^2}{x_1^2}}\right)\right],\quad (x_1\geqslant x_2),\tag{B8}$$

$$\frac{\partial}{\partial x_1}\det z_{12}=a(\det z_{12})\frac{1}{x_1+x_2}\Bigg[1-3x_1x_2-3x_1^2+3x_1^2(x_1+x_2)\tan^{-1}\frac{1}{x_1}-(1-x_1^2+x_2^2)\sqrt{\frac{1+x_2^2}{1+x_1^2}}-x_2(2x_1^2-x_2^2)E\left(\tan^{-1}\frac{1}{x_1},\sqrt{1-\frac{x_1^2}{x_2^2}}\right)+x_1^2x_2F\left(\tan^{-1}\frac{1}{x_1},\sqrt{1-\frac{x_1^2}{x_2^2}}\right)\Bigg],\quad (x_2\geqslant x_1),\tag{B9}$$

$$\frac{\partial}{\partial x_2}\det z_{12}=a(\det z_{12})\frac{1}{x_2+x_1}\Bigg[1-3x_2x_1-3x_2^2+3x_2^2(x_2+x_1)\tan^{-1}\frac{1}{x_2}-(1-2x_2^2+2x_1^2)\sqrt{\frac{1+x_2^2}{1+x_1^2}}-x_2(2x_2^2-x_1^2)E\left(\tan^{-1}\frac{1}{x_1},\sqrt{1-\frac{x_1^2}{x_2^2}}\right)+x_2x_1^2F\left(\tan^{-1}\frac{1}{x_1},\sqrt{1-\frac{x_1^2}{x_2^2}}\right)\Bigg],\quad (x_2\geqslant x_1).\tag{B10}$$

APPENDIX C: MATRIX ELEMENT OF THE HAMILTONIAN WITH UNEQUAL CONSTITUENT QUARK MASSES

We here give detailed computation of the matrix element of the Hamiltonian (2.1) $\langle u_1|H|u_2\rangle$ along the same line as the one in the preceeding appendix. Using the explicit expression for the interstate density matrix $W_{12,\mathbf{p}}$, Eq. (4.11), for the kinetic part we have

$$\mathrm{Tr}[\gamma^5\boldsymbol{\Sigma}\cdot\mathbf{p}W_{12,\mathbf{p}}]=-2\frac{E_{1\mathbf{p}}M_2+E_{2\mathbf{p}}M_1}{M_1+M_2}\theta(\Lambda^2-p^2).\tag{C1}$$

The direct terms of the interaction part are calculated as

$$\mathrm{Tr}[\beta W_{12,\mathbf{p}}]=-2\frac{E_{1\mathbf{p}}-E_{2\mathbf{p}}}{M_1+M_2}\theta(\Lambda^2-p^2),\quad \mathrm{Tr}[\beta\gamma^5W_{12,\mathbf{p}}]=0,\tag{C2}$$

the first of which is nonzero but it reduces to the first of Eq. (A2) when $M_1=M_2=M$. The exchange terms of the interaction part are also computed as

$$\mathrm{Tr}[\beta(1)W_{12,\mathbf{p}_1}(1)\beta(2)W_{12,\mathbf{p}_2}(2)]=\Bigg[1+\frac{E_{1\mathbf{p}_1}-E_{2\mathbf{p}_1}}{M_1+M_2}\cdot\frac{E_{1\mathbf{p}_2}-E_{2\mathbf{p}_2}}{M_1+M_2}-\frac{\mathbf{p}_1\cdot\mathbf{p}_2}{\mathbf{p}_1^2\mathbf{p}_2^2}\Bigg(\frac{E_{1\mathbf{p}_1}M_2+E_{2\mathbf{p}_1}M_1}{M_1+M_2}\frac{E_{1\mathbf{p}_2}M_2+E_{2\mathbf{p}_2}M_1}{M_1+M_2}-\frac{E_{1\mathbf{p}_1}E_{2\mathbf{p}_1}-\mathbf{p}_1\cdot\mathbf{p}_1+M_1M_2}{M_1+M_2}\frac{E_{1\mathbf{p}_2}E_{2\mathbf{p}_2}-\mathbf{p}_2\cdot\mathbf{p}_2+M_1M_2}{M_1+M_2}\Bigg)\Bigg]\theta(\Lambda^2-p^2),\tag{C3}$$

$$\mathrm{Tr}[\beta(1)\gamma^5(1)W_{12,\mathbf{p}_1}(1)\beta(2)\gamma^5(2)W_{12,\mathbf{p}_2}(2)]=\Bigg[-1+\frac{E_{1\mathbf{p}_1}-E_{2\mathbf{p}_1}}{M_1+M_2}\frac{E_{1\mathbf{p}_2}-E_{2\mathbf{p}_2}}{M_1+M_2}+\frac{\mathbf{p}_1\cdot\mathbf{p}_2}{\mathbf{p}_1^2\mathbf{p}_2^2}\Bigg(\frac{E_{1\mathbf{p}_1}M_2+E_{2\mathbf{p}_1}M_1}{M_1+M_2}\frac{E_{1\mathbf{p}_2}M_2+E_{2\mathbf{p}_2}M_1}{M_1+M_2}+\frac{E_{1\mathbf{p}_1}E_{2\mathbf{p}_1}-\mathbf{p}_1\cdot\mathbf{p}_1+M_1M_2}{M_1+M_2}\frac{E_{1\mathbf{p}_2}E_{2\mathbf{p}_2}-\mathbf{p}_2\cdot\mathbf{p}_2+M_1M_2}{M_1+M_2}\Bigg)\Bigg]\theta(\Lambda^2-p^2).\tag{C4}$$

Performing the integration over $\mathbf{p}$, $\mathbf{p}_1$, and $\mathbf{p}_2$, then the matrix element of the Hamiltonian $H[W_{12}]$ defined by Eq. (A5) is given as

$$H[W_{12}]=\int d^3\mathbf{r}\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[\gamma^5\boldsymbol{\Sigma}\cdot\mathbf{p}W_{12,\mathbf{p}}]-g\int d^3\mathbf{r}\left(\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[\beta W_{12,\mathbf{p}}]\right)^2-2g\int d^3\mathbf{r}\left(\int\frac{d^3\mathbf{p}}{(2\pi)^3}\theta(\Lambda^2-p^2)\right)^2,\tag{C5}$$

which is calculated to be

$$H[W_{12}]=-2\left[\int \frac{d^3\mathbf{p}}{(2\pi)^3}\frac{E_{1\mathbf{p}}M_2+E_{2\mathbf{p}}M_1}{M_1+M_2}\theta(\Lambda^2-p^2)\right]V-g\left[-2\int \frac{d^3\mathbf{p}}{(2\pi)^3}\frac{E_{1\mathbf{p}}-E_{2\mathbf{p}}}{M_1+M_2}\theta(\Lambda^2-p^2)\right]^2 V$$
$$-2g\left[\int \frac{d^3\mathbf{p}}{(2\pi)^3}\theta(\Lambda^2-p^2)\right]^2 V. \tag{C6}$$

From Eq. (C6) thus we can get a final form of the matrix element of the Hamiltonian, i.e., Eq. (4.15).

Following Ref. [9], it is easy to prove that the matrix element of the Hamiltonian $\langle u_1(\theta)|H|u_2(\theta)\rangle$ is invariant when the S-det $|u_{1(2)}\rangle$ undergoes the chiral transformation generated by $\exp[i(\theta/2)\Sigma_{j=1}^N\gamma_j^5]$.

We can easily find

$$\langle u_1(\theta)|H|u_2(\theta)\rangle=\int d^3\mathbf{r}\Sigma_{\mathbf{p}}H[W_{12,\mathbf{p}}(\theta)]\prod_{\mathbf{p}}\det z_{12,\mathbf{p}}\theta(\Lambda^2-p^2)=H[W_{12}]\det z_{12}, \tag{C7}$$

where

$$W_{12,\mathbf{p}}(\theta)\equiv e^{i(\theta/2)\gamma^5}W_{12,\mathbf{p}}e^{-i(\theta/2)\gamma^5}=\frac{1}{2}\left(1+\beta(\theta)\frac{A_{\mathbf{p}}-B_{\mathbf{p}}}{A_{\mathbf{p}}+B_{\mathbf{p}}}-\gamma^5\frac{C_{\mathbf{p}}+D_{\mathbf{p}}}{A_{\mathbf{p}}+B_{\mathbf{p}}}\mathbf{\Sigma}\cdot\mathbf{p}-\beta(\theta)\gamma^5\frac{C_{\mathbf{p}}-D_{\mathbf{p}}}{A_{\mathbf{p}}+B_{\mathbf{p}}}\mathbf{\Sigma}\cdot\mathbf{p}\right)\theta(\Lambda^2-p^2),$$
$$\beta(\theta)\equiv e^{i(\theta/2)\gamma^5}\beta e^{-i(\theta/2)\gamma^5}=\beta\cos\theta+\beta\gamma^5(-i\sin\theta). \tag{C8}$$

In fact, we have successively

$$\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[e^{-(\theta/2)\gamma^5}\gamma^5 e^{i(\theta/2)\gamma^5}\mathbf{\Sigma}\cdot\mathbf{p}W_{12,\mathbf{p}}]=\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[\gamma^5\mathbf{\Sigma}\cdot\mathbf{p}W_{12,\mathbf{p}}], \tag{C9}$$

$$\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[e^{-i(\theta/2)\gamma^5}\beta e^{i(\theta/2)\gamma^5}W_{12,\mathbf{p}}]=\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[\beta e^{i(\theta/2)\gamma^5}W_{12,\mathbf{p}}e^{-i(\theta/2)\gamma^5}]=\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[\beta W_{12,\mathbf{p}}]\cos\theta, \tag{C10}$$

$$\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[e^{-i(\theta/2)\gamma^5}\beta\gamma^5 e^{i(\theta/2)\gamma^5}W_{12,\mathbf{p}}]=\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[\beta\gamma^5 e^{i(\theta/2)\gamma^5}W_{12,\mathbf{p}}e^{-i(\theta/2)\gamma^5}]=i\int\frac{d^3\mathbf{p}}{(2\pi)^3}\mathrm{Tr}[\beta W_{12,\mathbf{p}}]\sin\theta. \tag{C11}$$

Equation (C9) shows trivially the chiral invariance. On the other hand, from Eqs. (C10) and (C11) it turns out that the direct term in addition with contributions of the exchange terms becomes also invariant under the chiral transformation. This fact holds also in the case of $M_1=M_2=M$ which is already pointed out in Appendix A. As the consequence of the use of these results, thus we can prove that the expectation value of the NJL Hamiltonian (2.1) by the superposed wave function $c_1|u_1\rangle+c_2|u_2\rangle$ becomes invariant under the chiral transformation.

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