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Note

Inverse Relativistic Problem for the Bound Quark–Antiquark States

One gives a formulation of the *inverse problem* for determining particle mass and potential parameters from the experimental bound-state energies. The solution of the *straight problems*, on which the inverse one is based, is reached by the use of the core-spline method. An autoregularized iteration process of Gauss–Newton type is applied for the solution of the overdetermined nonlinear system of equations, corresponding to the present formulation of the inverse problem. The concrete subjects of investigation are the mass and the coupling constant of the charmed quarks, whose boundstates are interpreted as masses of heavy vector mesons.

INTRODUCTION

The interpretation of the masses of the experimentally observed heavy vector mesons as quark–antiquark bound states makes possible the formulation of the inverse problem of determination of the quark mass and other basic parameters of the quark–antiquark interaction. For this purpose in the present paper we use the relativistic radial equation of the Todorov quasipotential approach [1]. We employ the potential proposed in Ref. [2].

Three formulations of the inverse problem are considered: (P_1)—based on the Schrödinger equation as in Ref. [2]; (P_2) and (P_3)—based on Eq. [1] for spin 1/2 relativistic quarks but using different approximations of the dominant interaction. The core-spline method [3, 4] is used for the solution of the mentioned radial equations (straight problems). The overdetermined nonlinear systems of equations with respect to the quark mass, m, and the coupling constant, λ, taking place in the inverse poblem are solved by means of autoregularized processes of Gauss–Newton type [5].

The present paper provides the necessary information about the employed computational methods and programs. Further, the values of m and λ obtained by solving the different formulations, (P_1)–(P_3), of the inverse problem of the energies of the charmonium bound states are compared.

1. THE STRAIGHT PROBLEM AND THE CORE-SPLINE METHOD

The straight problems, corresponding to the inverse problems (P_1)–(P_3) can be written compactly in the form

$$\left[\frac{d^2}{dx^2}+\frac{2(l+1)}{x}\frac{d}{dx}+b_v(z,m)-V_v(x;z;m,\lambda)\right]y(x,z)=0, \qquad (1.1)$$

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$$\int_0^\infty [x^{l+1}y(x, z)]^2\, dx = 1 \qquad (0 < x < \infty), \tag{1.2}$$

where index $v = 1, 2, 3$ corresponds to formulations (P_1)–(P_3), respectively; $b_1 = mz$, $b_2 = b_3 = (z^2 - 4m^2)/4$; $l = 0, 1, 2,...$ is the orbital quantum number; V_v is given potential (in case $v = 1$) or quasipotential (in cases $v = 2, 3$), depending on the particle mass m, on a constant λ and, generally, on the energy z.

The general features and the solution of problem (1.1), (1.2) by the core-spline method (CSM) is considered in detail in Refs. [3], [4, Sect. 1]. Our problem (1.1), (1.2) is a particular case of the general one [4, (1.1), (1.2), (1.4)–(1.7)]: this is the case of equal particle masses $m_1 = m_2 = m \in M = (0, m_b)$, $m_b = \text{constant} > 0$. Potential function V_v in (1.1) depends only on one parameter $\lambda \in L = (0, \lambda_b)$, $\lambda_b = \text{constant} > 0$ and it is constructed by making use of the potential introduced in Ref. [2],

$$V = C_1\{\lambda^2 x - [1 - 4I_{-1}(\lambda x)]/x\}, \tag{1.3}$$

where $C_1 = 8\pi/(33 - 2C_2)$, C_2 is an integer constant and I_{-1} is a particular case of the integrals

$$I_i(\lambda x) = \int_1^\infty \frac{\mu^i e^{-\lambda x \mu}}{\pi^2 + [\ln(\mu^2 - 1)]^2}\, d\mu \qquad (i = 0, \pm 1,...). \tag{1.4}$$

The core-spline method, when used to obtain approximate solutions of the straight problem (1.1), (1.2), consists of the determination of pairs: energy-wave function (see [3, p. 925; 4, (1.3)])

$$(\tilde{z}, \tilde{y}(x, \tilde{z})) \in Z \times \tilde{F}_p(X),$$

where $X = [x_a, x_b] \subset (0, \infty)$ and $Z = [z_a, z_b] \in R^1$ are given finite intervals (x_a is chosen to be close enough to zero and x_b as a large enough number [3, p. 934]; $\tilde{F}_p(X) = \{s(x)\ p(x, z)\}$, where $s(x)$ is a quadratic interpolation spline [3, (1.1)–(1.4)] and $p(x, z)$ is a core-function [3, p. 925]. The form of the core-function for equations of type (1.1) with potential (1.3) is fixed in Ref. [4, (1.9), (1.12)]

$$p(x, z) = \exp(-k_v(z)\, x^q) \qquad (v = 1, 2, 3),$$

where $q = 1.5$. The concrete form of function, k_v, as well as the length of the energy interval Z, depend on the details of the potential function V_v. Therefore, one has in different formulations of the problem

(i) *in the case* $v = 1$

$$V_1 = mV, \qquad k_1 = \lambda(C_1 m)^{1/2}/q, \qquad Z = (0, \infty);$$

(ii) *in the case* $v = 2$

$$V_2 = 2E_1 V, \qquad E_1 = (z^2 - 2m^2)/(2z),$$

$$k_2 = \lambda(2C_1 E_1)^{1/2}/q, \qquad Z = (\sqrt{2}\, m, \infty);$$

(iii) *in the case* $v = 3$

$$V_3 = V_2 + C_1\lambda^2\{E_2[1 + 2I_1(\lambda x)] + \lambda^2 E_3 I_3(\lambda x)\}/x,$$

$$E_2 = \frac{3z + 2m}{z(z + 2m)}, \qquad E_3 = \frac{2}{z(z + 2m)^2}, \qquad k_3 = k_2$$

and interval Z is the same as in the case $v = 2$.

According to Theorem 1 [3] the approximate solution of problem (1.1), (1.2) is reduced to the solution (with respect to the energy z) of the following nonlinear algebraic equation [4, (1.26)]

$$f(z; m, \lambda) \equiv 2\alpha_N^* + 2\left(\frac{l+1}{x_b} - qx_b^{q-1}k_v\right)(2\alpha_N^* x_b + \beta_N^*)$$
$$+ [b_v - q(2l + q + 1)\, x_b^{q-2}k_v - V_v(x_b) + q^2 x_b^{2(q-1)}k_v^2]$$
$$\times (\alpha_N^* x_b^2 + \beta_N^* x_b + \gamma_N^*) = 0 \qquad (v = 1, 2, 3), \tag{1.5}$$

where $N \geqslant 5$ is the number of spline-net intervals; α_N^*, β_N^*, γ_N^* are the basic-spline coefficients [3, (1.4), (1.8), (1.11), (1.15), (1.17)]. Quantities α_N^*, β_N^*, γ_N^*, k_v, b_v and V_v depend generally on the variables z, m, λ and the number l.

The sufficient conditions for applicability of Theorem 1 [3] and, therefore, for construction of a basic spline in CSM are given in Refs. [3, (1.9), (1.13); 4, (1.23)–(1.25)]. These conditions can be checked analytically only in a few cases of special potentials and, usually, the question of applicability of Theorem 1 [3] is solved by numerical experiments.

2. On the Choice of the Relativistic Quasipotential Function

The choice of the functions V_2 and V_3 is based on the quantum chromodynamics at short distances. We assume Lagrangian of quantum chromodynamics to be invariant with respect to the $SU(3)_c \otimes SU(4)_f$, where the indices "c" and "f" denote a colour and a flavour of the quarks, respectively. The potential function $\tilde{V}(\underline{p}, \underline{q})$ is extracted from the Born spin 1/2 quark–antiquark interaction amplitude for $SU(3)_c$-singlet initial and final states.

The potential written in a two-component formalism by means of the Pauli matrices has in momentum space the form

$$\tilde{V}(p,q) = -\frac{16\pi}{3}\frac{\alpha_s}{(p-q)^2}[2z^2 - 4m^2 - (p-q)^2]$$
$$+\frac{16\pi}{3}\alpha_s\left[\frac{2z}{z+2m} - \frac{(p-q)^2}{(z+2m)^2}\right]$$
$$-i\frac{32\pi}{3}\frac{\alpha_s}{(p-q)^2}\left[1 + \frac{z}{z+2m} - \frac{(p-q)^2}{(z+2m)^2}\right][(p*q)\sigma_1 + (p*q)\sigma_2]$$
$$+\frac{16\pi}{3}\alpha_s\left[\delta_{jj'} - \frac{(p*q)_j(p*q)_{j'}}{(p-q)^2}\right.$$
$$\left.+\frac{4}{(z+2m)^2}\cdot\frac{(p*q)_j(p*q)_{j'}}{(p-q)^2}\right]\sigma_{1j}\sigma_{2j'}, \qquad i \equiv \sqrt{-1}, \tag{2.1}$$

where $p \equiv p_1$ $(=-p_2)$ and $q \equiv q_1$ $(=-q_2)$ are the momenta of the initial and, respectively, final particles in the center-of-mass frame, z is the total center-of-mass energy, σ_{1j} and $\sigma_{2j'}$ are two sets of Pauli matrices, commuting one with the other and

$$\alpha_s = \frac{12\pi}{33 - 2C_2}\left[\ln\left(\frac{(p-q)^2}{\lambda^2}\right)\right]^{-1}, \tag{2.2}$$

where λ is a scale parameter.

Formula (2.2) takes into account the vacuum polarization effects and it is the solution of the renormalization group equation at the large space-like momentum transfers.

In order to account for the nonperturbative effects at short distances instead of formula (2.2) we shall make use of the expression proposed in Ref. [2]:

$$\alpha_s = \frac{12\pi}{33 - 2C_2}\left[\ln\left(1 + \frac{(p-q)^2}{\lambda^2}\right)\right]^{-1}. \tag{2.3}$$

Formula (2.3) simultaneously satisfies the requirements for asymptotic freedom at short distances and linear increase of the strength of the interaction at large distances.

In the case $\nu = 2$ (the formulation of the problem (P_2)) we use only the first term in the right-hand side of (2.1) (the Coulomb term). Then Eq. (1.1) differs from the nonrelativistic Schrödinger equation for spinless quarks (the case $\nu = 1$) only by the functions b_2 and V_2 depending on z.

In the case $\nu = 3$ (the formulation (P_3)) we use all the diagonal terms in the right-hand side of (2.1), i.e., the first four terms. The conjecture is that the spin-orbit and spin-spin interaction terms in the right-hand side of (2.1) do not contribute substantially.

The functions V_ν $(\nu = 2, 3)$ in the co-ordinate space are obtained from the approximations for $\tilde{V}(p,q)$ (see formula (2.1)) by a Fourier transformation. The integration is carried out by making use of a spectral representation of the integrands. In the present work we choose $C_2 = 3$.

3. Inverse Problem

Let a point $P^* = (z^*, m^*, \lambda^*) \in Z \times M \times L$ that satisfies Eq. (1.5) be given. The derivatives $\partial f(z, m, \lambda)/\partial r$, where $r = z, m, \lambda$ have the form

$$\begin{aligned}\frac{\partial f}{\partial r} &= 2\frac{\partial \alpha_N^*}{\partial r} - 2qx_b^{q-1}\frac{\partial k_v}{\partial r}(2\alpha_N^* x_b + \beta_N^*) \\ &+ 2\left(\frac{l+1}{x_b} - qx_b^{q-1}k_v\right)\left(2\frac{\partial \alpha_N^*}{\partial r}x_b + \frac{\partial \beta_N^*}{\partial r}\right) \\ &+ \left[\frac{\partial b_v}{\partial r} - q(2l+q+1)\,x_b^{q-2}\frac{\partial k_v}{\partial r} - \frac{\partial V_v}{\partial r}\right|_{x=x_b} \\ &+ 2q^2 x_b^{2(q-1)}k_v\frac{\partial k_v}{\partial r}\Bigg](\alpha_N^* x_b^2 + \beta_N^* x_b + \gamma_N^*) \\ &+ [b_v - q(2l+q+1)\,x_b^{q-2}k_v - V_v(x_b) \\ &+ q^2 x_b^{2(q-1)}k_v^2]\left(\frac{\partial \alpha_N^*}{\partial r}x_b^2 + \frac{\partial \beta_N^*}{\partial r}x_b + \frac{\partial \gamma_N^*}{\partial r}\right), \qquad v = 1, 2, 3.\end{aligned}$$

Let, also, the derivative $\partial f/\partial r$ be continuous at the point P^* and the following inequality holds:

$$\frac{\partial f}{\partial z} \neq 0. \tag{3.1}$$

Then the theorem about implicit function in the neighbourhood of the point P^* implies the existence of a differentiable function

$$z = z(m, \lambda) \tag{3.2}$$

with partial derivatives

$$\frac{\partial z}{\partial m} = -\frac{\partial f}{\partial m}\Big/\frac{\partial f}{\partial z} \qquad \text{and} \qquad \frac{\partial z}{\partial \lambda} = -\frac{\partial f}{\partial \lambda}\Big/\frac{\partial f}{\partial z}.$$

The existence of the implicit function (3.2) gives the possibility of considering the inverse problem of numerical determination of the parameters m and λ of the quark–antiquark system. For this purpose, suppose that the vector of the measured energies

$$\tilde{\mathbf{z}} = (\tilde{z}_{0,0}, \ldots, \tilde{z}_{0,\mu^{(0)}}, \tilde{z}_{1,0}, \ldots, \tilde{z}_{1,\mu^{(1)}}, \tilde{z}_{l^*,0}, \ldots, \tilde{z}_{l^*,\mu^{(l^*)}})^T \in R^s,$$
$$s = \mu^{(0)} + \mu^{(1)} + \cdots + \mu^{(l^*)}, \qquad l^* = \text{const.} \geqslant 0,$$

is given, and its components $\tilde{z}_{l,\mu^{(l)}} \in Z$ are labeled by two indices: the orbital quantum number l and the corresponding radial numbers $\mu^{(l)}$. Suppose further that the implicit function (3.2) determines a corresponding vector

$$\mathbf{z}(\psi) = (z_{0,0}(\psi),..., z_{0,\mu^{(0)}}(\psi),..., z_{l^*,0},..., z_{l^*,\mu^{(l^*)}})^T \in R^s,$$
$$\psi = (m, \lambda)^T \in R^2,$$

whose components are the energies $z_{l,\mu^{(l)}} \in Z$ approximately computed by the core-spline method. Note that the core-spline method holds under conditions that provide a considerably smaller error of the components of the vector $\mathbf{z}$ with respect to the error of the components of the measured vector $\tilde{\mathbf{z}}$.

The minimization of the functional $\chi^2(\psi) = \| w(\mathbf{z}(\psi) - \tilde{\mathbf{z}}) \|_2^2$, where w is a given diagonal weighing matrix of the order s, leads to the solution of a $(\mathbf{z}'(\psi)w)^T$-averaged equation [7]

$$\Phi(\psi) = (\mathbf{z}'(\psi))^T w^2(\mathbf{z}(\psi) - \tilde{\mathbf{z}}) = 0 \tag{3.3}$$

with respect to the vector ψ. The symbol $\mathbf{z}'(\psi)$ in Eq. (3.3) stands for the Jacobi matrix of the vector $\mathbf{z}(\psi)$

$$\mathbf{z}'(\psi) = \begin{bmatrix} \dfrac{\partial z_{0,0}}{\partial m} & \cdots & \dfrac{\partial z_{l^*,\mu^{(l^*)}}}{\partial m} \\ \dfrac{\partial z_{0,0}}{\partial \lambda} & \cdots & \dfrac{\partial z_{l^*,\mu^{(l^*)}}}{\partial \lambda} \end{bmatrix}$$

The system of two equations (3.3) for the two unknowns m and λ is considered as the *inverse quark–antiquark bound states problem.* In order to solve this problem, the present paper uses the *autoregularized iteration process of Gauss–Newton type*

$$\psi_{n+1} = \psi_n - ((\mathbf{z}'(\psi_n))^T w^2 \mathbf{z}'(\psi_n) + \varepsilon_n I_{Rs})^{-1} \Phi(\psi_n),$$
$$\psi_n \in M \times L, \quad n = 0, 1,..., n^*, \tag{3.4}$$

where I_{Rs} is unit matrix of order s. The autoregularizer ε_n has the form [9]

$$\varepsilon_n = [(\tau_n^2 + 4C\rho_n)^{1/2} - \tau_n]/2,$$
$$\tau_n = \| (\mathbf{z}'(\psi_n))^T w^2 \mathbf{z}'(\psi_n) \|_\infty, \qquad \rho_n = \| \Phi(\psi_n) \|_\infty,$$
$$C = \varepsilon_0(\varepsilon_0 + \tau_0)/\rho_0, \qquad \varepsilon_0 = \text{const.} > 0.$$

Practically, the components of the vector $\mathbf{z}(\psi)$ are generated by the program SPSOL [4, 8], while the iteration process (3.4) is executed by the standard program COMPIL (Program Library of JINR, Dubna; program No. C-401). The latter one is based on the basic program REGN [9]. (New version: PSR-165/REGN, ORNL-RSIC-31.)

4. Solution of the Inverse Problem for the Charmonium Bound States

In order to solve problem (3.3) we consider the measured vector to be the seven-component vector

$$\tilde{\mathbf{z}} = (\tilde{z}_{0,0}, \tilde{z}_{0,1}, \tilde{z}_{0,2}, \tilde{z}_{0,3}, \tilde{z}_{1,0}, \tilde{z}_{2,0}, \tilde{z}_{2,1})^T,$$

which is obtained from the vector $\mathcal{M}$ of measured masses (in GeV) of the bound states of the quark–antiquark [6]

$$\mathcal{M} = ((3.098)_{0,0}, (3.684)_{0,1}, (4.028)_{0,2}, (4.414)_{0,3}, (3.522)_{1,0}, (3.772)_{2,0}, (4.16)_{2,1})^T.$$

The components of both vectors are connected by the relations

$$\tilde{z}_{l,\mu(l)} = \mathcal{M}_{l,\mu(l)} - 2m, \quad \text{for} \quad \nu = 1, \tag{4.1}$$

$$\tilde{z}_{l,\mu(l)} = (\mathcal{M}_{l,\mu(l)})^{1/2}, \quad \text{for} \quad \nu = 2, 3.$$

The problems (P_1)–(P_3) were solved in two steps,

(a) With a unit weighing matrix $w = I_R s$;

(b) With $w = \text{diag}(|z_{0,0}(\psi_{n^*}) - \tilde{z}_{0,0}|^{-1/2}, \ldots, |z_{2,1}(\psi_{n^*}) - \tilde{z}_{2,1}|^{-1/2})$, where ψ_{n^*} is a n^*-pseudo-soution [7], found by the iteration process (3.4) in step (a). The second step, (b), consists of the application of the LCH-procedure [10].

The iteration process applied to all variants of problem (3.3) is cut off at the number n^* for which the inequality

$$\rho_{n^*} \leqslant 10^{-11} \tag{4.3}$$

is satisfied.

In order to compute the energies $z_{l,\mu(l)}$ the subroutine SPSOL [8] that realizes the core-spline method for all problems (1.1), (1.2) is called by the subroutine RELADI [9]. The program SPSOL was used in all cases at equal values of the parameters: $N = 400$, $X = [10^{-7}, 10]$. Such a regime provides an accuracy $(\Delta z)_{\text{low}} = 7.4 \times 10^{-6}$ of the computed energies (see [4, (2.8)]) of the order higher than the accuracy of the vector $\tilde{\mathbf{z}}$ components of the measured energies. The integrals (1.4) were computed by means of the Gauss four-point formula. The iteration process was realized by a numerical approximation of the Jacobi matrix (see [9, p. 17]). An alternative of the numerical differentiation is the use of formulae for the derivatives $\partial z/\partial m$ and $\partial z/\partial \lambda$, which are guaranteed by the implicit function theorem (see Section 3).

The results from the two steps (a) and (b) of the procedure of solving the inverse problems (P_1)–(P_3) are listed in Table I. In the same table are also listed the values of the statistical criterion $\chi^2(\psi_{n^*})/(s-2)$ corresponding to the solution of the problems

TABLE I

Quark Mass and Coupling Constant Obtained at Both Steps of Solution of the Inverse Problem

		$\nu = 1$	$\nu = 2$	$\nu = 3$	Results of Ref. [2]
Step (a)	m (GeV)	1.50432 ± 0.013	1.57943 ± 0.018	1.56547 ± 0.022	1.491
	λ (GeV)	0.38462 ± 0.0064	0.31841 ± 0.0071	0.31961 ± 0.0081	0.398
Step (b)	m (GeV)	1.49976 ± 0.0056	1.59033 ± 0.0089	1.58848 ± 0.0155	
	λ (GeV)	0.38726 ± 0.0024	0.31505 ± 0.0034	0.31246 ± 0.0053	
	$\frac{\chi^2(\psi_{n^*})}{s-2}$	1.1005174	1.0362254	0.974156	

(P_1)–(P_3) at step (b). This criterion allows comparison of the abilities of the three formulations ($\nu = 1, 2, 3$) to describe the quark–antiquark system on the basis of Eq. (1.1). The best formulation corresponds to such value of the quantity $\chi^2(\psi_{n^*})/(s-2)$ which is closer to unity.

The results in Table I first of all indicate an advantage in the relativistic equations (1.1) ($\nu = 2, 3$) with respect to the Schrödinger equation. Particularly, it is clear that the relativistic equation (1.1) with a more complete quasipotential V_3 has an advantage with respect to Eq. (1.1) with "Coulomb" quasipotential V_2.

The approach chosen to formulate and solve inverse problem (3.3), the latter being obtained by consideration of an overdetermined system of equations (consisting of seven equations for two unknown quantities), allows estimation of the inherited errors of the unknown quantities m and λ. For this purpose the matrix $[(\mathbf{z}'(\psi_{n^*}))^T w\mathbf{z}(\psi_{n^*})]^{-1}$ which appeared to be well-conditioned, was used as the Fischer information matrix. The errors listed in Table I are extracted from this

TABLE II

Charmonium Masses $\mu_{l,\mu}$ (in GeV) Calculated by the Values of m and λ, Obtained from the Inverse Problem

l	μ	$\nu = 1$	$\nu = 2$	$\nu = 3$
0	0	3.0989	3.1868	3.2175
	1	3.6696	3.6428	3.6577
	2	4.0675	4.0467	4.0517
	3	4.4143	4.4233	4.4210
	4*	4.8060	4.7915	4.7852
	5*	5.3177	5.1804	5.1733
1	0	3.5056	3.5062	3.5116
2	0	3.7816	3.7732	3.7707
	1	4.1420	4.1524	4.1438
	2*	4.4679	4.5136	4.5000
	3*	4.8395	4.8715	4.8552

matrix. We note that the breaking of the iteration process (3.4) according to criterion (4.3) promotes more plausible application of the linear theory of the inherited errors in the considered nonlinear case.

Finally, the results in Table I indicate the presence of a clearly demonstrated relativistic effect, even for such relatively heavy quarks as the charmed quarks. The relativistic value of the quark mass is ~4% larger than the classical one and the relativistic value of the quantity λ is ~16% smaller than the value of the classical charmonium treatment.

The charmonium masses $M_{l,\mu(l)}$ computed by the CSM (function (3.2) and formulae (4.1), (4.2) are used) and corresponding to the solution $\psi_{n^*}^{(\nu)}$ ($\nu = 1, 2, 3$) obtained at step (b) (Table I), are listed in Table II. The predicted values of the masses are noted by the symbol (*).

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