Sign ambiguity in configuration mixing and coupled channel calculations

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(Received 2 August 1995; revised manuscript received 13 March 1996)

In this paper we discuss the problem of sign ambiguity, which is common both to first and second order configuration mixing in structure calculations, as well as to the coupled channel method for scattering problems. The sign ambiguity propagates into reduced matrix elements and/or into scattering amplitudes; the assertion that these quantities can be extracted from data analysis, including their signs, in order to be compared with theoretical models, is incorrect. The measurable quantities, as derived from density matrix, are insensitive to both initial and succesive sign changes in the calculations. [S1063-651X(96)10907-7]

PACS number(s): 02.70.−c, 21.60.−n, 24.10.Eq, 03.65.Ge

The aim of this paper is to discuss the problem of sign ambiguity, specific to computational methods used in nuclear structure configuration mixing and coupled channel calculations. The wave functions resulting from configuration mixing have an overall sign ambiguity. The numerical results as transition operator matrix elements, channel coupling elements or S-matrix elements conserve the sign ambiguity resulting from configuration mixing calculations, but the density matrix is free from sign ambiguity.

In configuration mixing calculations one has to solve a homogeneous system of linear equations in order to find the amplitudes of the wave functions in a given basis, e.g., [1]. The solution of a system of N linear equations is determined up to an arbitrary multiplicative constant, provided its rank is $N-1$, e.g., [2]. The magnitude of this constant can be fixed by the normalization condition (the sum of the squared amplitudes must be unity), but not its sign. This is the sign ambiguity for configuration mixing calculations met in nuclear structure studies; the well-known example is the configuration mixing for two states, e.g., [1]. The wave functions resulting from this procedure are determined up to an overall $(\pm)$ sign. It should be evinced that the magnitudes as well as the relative signs of the wave-function components (amplitudes) are calculated correctly.

In usual, say, first-order, configuration mixing calculations, the basis vectors are defined including their signs; examples of such basis vectors could be the unperturbed single-particle states in shell-model calculations [1], or SU(5) basis vectors in the interacting boson model [3]. In second-order configuration mixing calculations, one uses as basis vectors the wave functions obtained in first-order mixing calculations [3]; the vectors of this basis, obtained up to an overall sign, can have flipped signs. If the vectors i,j,k have the signs changed, this will result in changed signs of the rows and columns labeled by i,j,k in the Hamiltonian matrix. The new system of homogeneous linear equations is equivalent to the system with correct signs, provided the amplitudes labeled by the indices i and j and k change their signs too. As a result, the products of amplitudes by the corresponding basis vectors have correct signs, irrespective of whether basis vectors did or did not have initially correct signs. The relative signs between the components (amplitudes multiplying basis vectors) of the wave functions, resulting from a second-order configuration mixing, remain unaltered. The wave functions obtained in second order configuration mixing calculations are, as in first order calculations, determined up to an overall sign.

The sign ambiguity appearing in the description of the nuclear structure will be illustrated in the case of the interacting boson model (IBM) for the ^{112}Cd nucleus. We use a configuration mixing IBM-2 calculations [4] with typical parameters taken from literature [5], our goal being only to illustrate the sign ambiguity and not to compare the calculations with experimental data.

The calculations are carried out in two steps. In the first step the Hamiltonian H is diagonalized for each configuration separately in the usual SU(5) basis,

$$H=\epsilon_\pi d_\pi^\dagger\cdot\tilde{d}_\pi+\epsilon_\nu d_\nu^\dagger\cdot\tilde{d}_\nu+V_{\pi\pi}+V_{\nu\nu}+kQ_\pi\cdot Q_\nu+M_{\pi\nu}, \tag{1}$$

where

$$V_{\rho\rho}=\sum_{L=0,2,4}\frac{1}{2}\,c_{L\rho}\sqrt{2L+1}[(d_\rho^\dagger d_\rho^\dagger)^{(L)}\cdot(\tilde{d}_\rho\tilde{d}_\rho)^{(L)}]^{(0)}$$

and

$$Q_\rho=(s_\rho^\dagger\tilde{d}_\rho+d_\rho^\dagger s_\rho)^{(2)}+\chi(d_\rho^\dagger\tilde{d}_\rho)^{(2)} \tag{2}$$

are the quadrupole operators with $\rho=\pi,\nu$. In the second step $H+H_{\mathrm{mix}}$ is diagonalized in a basis provided by the four lowest eigenstates of the two configurations where

$$H_{\mathrm{mix}}=\alpha(s_\pi^\dagger s_\pi^\dagger+s_\pi s_\pi)^{(0)}+\beta(d_\pi^\dagger d_\pi^\dagger+\tilde{d}_\pi\tilde{d}_\pi)^{(0)}. \tag{3}$$

TABLE I. Reduced matrix elements of quadrupole operators between the unmixed eigenstates of first configuration; effect of the sign change for 0(2) and 2(2).

$I_i(n)$	$I_f(m)$	$(s^\dagger\tilde{d}+d^\dagger s)^{(2)}_\nu$	$(d^\dagger\tilde{d})^{(2)}_\nu$	$(s^\dagger\tilde{d}+d^\dagger s)^{(2)}_\pi$	$(d^\dagger\tilde{d})^{(2)}_\pi$
2 (1)	0 (1)	-6.3010	0.0875	-1.1730	0.0406
		-6.3010	0.0875	-1.1730	0.0406
2 (1)	0 (2)	-3.1303	0.3143	-0.3119	0.0751
		3.1303	-0.3143	0.3119	-0.0751
2 (1)	0 (3)	0.2524	0.2172	0.0445	0.0666
		0.2524	0.2172	0.0445	0.0666
2 (1)	0 (4)	0.0680	0.0418	-0.0920	0.0416
		0.0680	0.0418	-0.0920	0.0416
2 (2)	0 (1)	0.8026	0.4970	0.1772	0.1645
		-0.8026	-0.4970	-0.1772	-0.1645
2 (2)	0 (2)	-1.2481	1.7188	-0.3116	0.2051
		-1.2481	1.7188	-0.3116	0.2051
2 (2)	0 (3)	-3.8962	-0.3056	-0.5387	-0.0867
		3.8962	0.3056	0.5387	0.0867
2 (2)	0 (4)	-0.3838	-0.2488	-0.1039	0.0395
		0.3838	0.2488	0.1039	-0.0395

The eigenstates obtained in the first step or in the second step were used to evaluate the reduced matrix elements for the multipole operators and in particular for the quadrupole operators (2). The reduced matrix elements of the multipole operators can be used to describe the electromagnetic transitions or they give reduced matrix elements in the transition potential for the coupled-channel analysis of nuclear reactions [6] or for the Coulomb excitation analysis [7].

The real normalized solutions are determined up to a sign in the SU(5) basis. The arbitrariness is due to the numerical method as there are no physical arguments to choose the signs. Therefore we consider the lowest four eigenstates of the Hamiltonian (1) for $L=0,\ 2$, and 4 in the two configurations. To see the effects of the sign ambiguity we change the signs of the second eigenstates for $L=0,\ 2$, and 4 in the first configuration.

First we use the original and the sign changed eigenstates, respectively, to evaluate the following reduced matrix elements (see Table I):

$$\langle I_i(n)||(d^\dagger\tilde{d})^{(2)}_\rho||I_f(m)\rangle,$$

$$\langle I_i(n)||(s^\dagger\tilde{d}+d^\dagger s)^{(2)}_\rho||I_f(m)\rangle. \tag{4}$$

One observes that the signs of the reduced matrix elements depend on the relative sign of the wave functions $|I_i(n)\rangle$ and $|I_f(m)\rangle$.

The original (''standard'') and sign changed eigenstates obtained diagonalizing the Hamiltonian (1) were used to diagonalize the mixing Hamiltonian in the direct sum of the basis of the two configurations (see Table II).

One may observe that the components of the mixed wave functions that belong to the second unmixed eigenstates of the first configuration change the sign. Moreover, the seventh mixed eigenstate with $L=0$ and the fifth mixed eigenstate with $L=2$ or $L=4$ acquire a global sign change.

The mixed eigenstates mentioned above [''standard'' and with sign changed for $0(7)$, $2(5)$, and $4(5)$] were used to evaluate the reduced matrix elements (4).

As we can see in Table III, the signs of the reduced matrix elements depend on the relative sign of the wave functions $|I_i(n)\rangle$ and $|I_f(m)\rangle$.

To conclude, there is no physical argument to fix the signs of the wave functions in the IBM calculations. This ambiguity results in a sign ambiguity for the reduced matrix elements of the multipole operators. This means that only the relative signs of the reduced matrix elements of the multipole operators have a physical meaning and not their particular values. The conservation of relative signs of the reduced matrix elements of the multipole transition operators is of vital importance because the (constructive or destructive) interference depends on the relative signs of the terms in the wave functions.

TABLE II. Eigenstates of the mixing Hamiltonian in the unmixed basis; effect of the sign change for 0(2) and 2(2) in first configuration.

$I(n)$	Energies	Amplitudes of first configuration				Amplitudes of second configuration			
0(1)	0.0000	0.9967	0.0052	-0.0016	-0.0002	0.0676	-0.0064	0.0440	-0.0029
		0.9967	-0.0052	-0.0016	-0.0002	0.0676	-0.0064	0.0440	-0.0029
0(2)	1.2419	0.0426	-0.8240	0.0248	0.0270	-0.5589	0.0734	0.0037	-0.0097
		0.0426	0.8240	0.0248	0.0270	-0.5589	0.0734	0.0037	-0.0097
0(6)	2.5740	-0.0192	-0.0105	-0.0159	0.9251	0.0478	-0.0866	0.3596	0.0656
		-0.0192	0.0105	-0.0159	0.9251	0.0478	-0.0866	0.3596	0.0656
0(7)	2.8285	-0.0405	0.0014	0.0132	-0.3562	-0.0116	0.0224	0.9316	-0.0528
		0.0405	0.0014	-0.0132	0.3562	0.0116	-0.0224	-0.9316	0.0528
0(8)	3.0455	-0.0020	0.0128	0.0287	0.0812	0.0033	0.0005	-0.0259	-0.9959
		-0.0020	-0.0128	0.0287	0.0812	0.0033	0.0005	-0.0259	-0.9959
2(1)	0.6433	-0.9932	0.0002	0.0083	0.0000	-0.1039	0.0524	-0.0004	0.0032
		-0.9932	-0.0002	0.0083	0.0000	-0.1039	0.0524	-0.0004	0.0032
2(5)	2.0050	0.0267	0.0427	-0.9163	0.0231	-0.1595	0.3322	-0.1459	0.0146
		-0.0267	0.0427	0.9163	-0.0231	0.1595	-0.3322	0.1459	-0.0146

TABLE III. Reduced matrix elements of quadrupole operators between the mixed eigenstates of Table II.

$I_i(n)$	$I_f(m)$	$(s^\dagger\tilde{d}+d^\dagger s)^{(2)}_\nu$	$(d^\dagger\tilde{d})^{(2)}_\nu$	$(s^\dagger\tilde{d}+d^\dagger s)^{(2)}_\pi$	$(d^\dagger\tilde{d})^{(2)}_\pi$
2(1)	0(1)	6.3234	-0.0866	1.1860	-0.0388
		6.3234	-0.0866	1.1860	-0.0388
2(1)	0(2)	-2.8839	0.2381	-0.4310	0.0412
		-2.8839	0.2381	-0.4310	0.0412
2(1)	0(6)	-0.1846	-0.0417	0.0833	-0.0433
		-0.1846	-0.0417	0.0833	-0.0433
2(1)	0(7)	-0.2569	0.0040	-0.0784	0.0011
		0.2569	-0.0040	0.0784	-0.0011
2(1)	0(8)	-0.0141	-0.0101	0.0041	-0.0067
		-0.0141	-0.0101	0.0041	-0.0067
2(5)	0(1)	-0.6010	-0.0320	0.4295	-0.0242
		0.6010	0.0320	-0.4295	0.0242
2(5)	0(2)	3.2473	0.0631	0.4069	0.0340
		-3.2473	-0.0631	-0.4069	-0.0340
2(5)	0(6)	3.1663	-0.2346	0.4513	-0.0829
		-3.1663	0.2346	-0.4513	0.0829
2(5)	0(7)	-1.0541	0.3180	-0.0819	0.0362
		-1.0541	0.3180	-0.0819	0.0362
2(5)	0(8)	-0.0231	0.1912	0.0180	0.0628
		0.0231	-0.1912	-0.0180	-0.0628

Usually it is stated that this overall sign ambiguity of the wave functions has no physical consequences, as long as the wave functions differing in phase represent the same state. This assertion is true if we refer only to the magnitude of the matrix elements, as, for example, the transition probabilities. However, in some calculations one needs the matrix elements, including their signs, and not only their magnitudes. For example, in coupled channel calculations one needs the potential matrix elements $V_{mn}=\langle m|V|n\rangle$. If the wave function of the state m is affected by the sign ambiguity, this propagates to the row m, V_{mn}, and to the column m, V_{nm}, of the potential matrix. In the next step one has to solve a system of coupled Schrödinger equations, whose potential matrix has a sign ambiguity for both column m and row m. The regular solution of the system consists in N independent solutions X_{mn} $(m,n=1,2,3,\ldots,N)$, where N is the number of the involved channels [8]. The sign ambiguity in the potential matrix results in sign ambiguity of the solution matrix $X=||X_{mn}||$; both row and column m are affected. This property holds also for the logarithmic derivative of the solution $R=X'X^{-1}$ (X' is the derivative matrix). Indeed, for a system of coupled Schrödinger equations

$$X''+(V-E)X=0, \quad E=||E_l\delta_{ln}||$$

the logarithmic derivative R is a solution of the Ricatti matrix equation

$$R'+(V-E)+R^2=0.$$

One can verify with this equation that if V changes signs in the column and row m, so does the solution R. Now, with the logarithmic derivative matrix R one constructs, in the asymptotic region, the S matrix

$$S=[RH^{(+)}-H^{(+)\prime}]^{-1}[RH^{(-)}-H^{(-)\prime}],$$

where $H^{(+)}$, $H^{(-)}$, $H^{(+)\prime}$, $H^{(-)\prime}$ denote the diagonal matrices of the out and in waves and their derivatives, respectively. The change of signs of the row and column m in the R matrix will result in a change of sign of the same row and column in the S matrix. All S-matrix elements S_{mn} and S_{nm} (m fixed, $n\neq m$) connecting the channel (target nucleus state) m with other channels n, change their sign, irrespective of the other quantum numbers labeling the channels (total angular momentum, orbital momenta in channels m and n). The transition amplitude from initial channel 0 to final channel f, T_{0f}, constructed with kinematical quantities (angular momentum coupling coefficients, spherical harmonics) and with S matrix elements (see, e.g., [8]), has the same sign ambiguity. The density matrix for a given final channel f, ρ_f, is constructed in terms of the density matrix for initial channel ρ_0 and bilinear combinations of the transition amplitudes terms, $\rho_f=T_{f0}\rho_0T^\dagger_{0f}$ is free of sign ambiguity. We conclude that the density matrix of final reactions channels and observables deriving from it (cross section, polarization) are not sensitive to sign ambiguity but that one cannot extract from measured density matrix the matrix elements of the transition operators including their signs. The inverse procedure of extracting reduced matrix elements from density matrix experimental data results in correct relative signs but remains, however, in an overall sign ambiguity.

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