Algebraic model for quantum scattering: Reformulation, analysis, and numerical strategies

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The convergence problem for scattering states is studied in detail within the framework of the algebraic model, a representation of the Schrödinger equation in an L^2 basis. The dynamical equations of this model are reformulated featuring new ''dynamical coefficients,'' which explicitly reveal the potential effects. A general analysis of the dynamical coefficients leads to an optimal basis yielding well converging, precise, and stable results. A set of strategies for solving the equations for nonoptimal bases is formulated based on the asymptotic behavior of the dynamical coefficients. These strategies are shown to provide a dramatically improved convergence of the solutions. [S1050-2947(96)02912-5]

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I. INTRODUCTION

In the quest for solving the Schrödinger equation for both bound and continuum states, square-integrable bases have been repeatedly used. For bound states this turns out to be a traditional way to obtain the spectral properties of quantum systems. It has been shown however that a single representation of the Schrödinger equation in terms of an L^2 basis can be formulated that allows for a description of both bound and continuum states [1–5].

A version of such a formulation is called the algebraic model of the resonating group method (hereafter, referred to as the algebraic model or AM). It was originally tailored to treat clusterized problems, but can be used for all kinds of quantum-mechanical many-particle configurations without major modifications. The AM has been formulated in terms of different types of bases, depending on the more specific features of the quantum system considered. One very important feature of the AM is the fact that the boundary conditions of the system are translated from a coordinate space context to the context of expansion coefficients, and are explicitly incorporated in the dynamical equations [1–4].

We will consider a specific AM formulation (i.e., a specific L^2 basis) to elucidate the analysis of the method. The methodology used for this analysis is of a general nature however, and can be repeated for other bases. The specific AM version chosen in this paper features an oscillator basis, and is, in particular, very suitable for obtaining both the bound and continuum spectra of nuclear systems with very different configurational properties; where appropriate, nuclear spectroscopic units will therefore be used. The choice of this AM version is mainly due to the background of the authors. Results of the AM approach considered here have already been reported on [6,7], and show, in particular, how the coupling of cluster and collective configurations can be treated seamlessly in such a description.

Where necessary, a specific form for the potential operator will be used. We will consider a Gaussian form in this work. Although this again is a popular potential form in nuclear spectroscopic calculations, it is also an interesting functional form to approximate a large variety of potentials by discrete and continuous superpositions.

We will concentrate our attention to the solutions of the dynamical equations for scattering situations only, as these are much more involved than the bound state problems. Indeed, the latter can be well approximated by a simple diagonalization of the energy matrix, as is well known.

We will specifically discuss how strongly the convergence of the solutions of an AM system depend on the parameters of the problem. In particular, the dependence on the precision and the convergence properties of the solutions of both the oscillator radius of the basis (the parameter unambiguously fixing the square-integrable basis) and the form of the potential energy contribution, will be treated in detail.

The convergence is crucial for obtaining stable approximations to the solutions of problems expressed in terms of an (infinite) set of basis functions, in our case an L^2 basis. This problem was repeatedly investigated, mainly for bound-state solutions. As applications to scattering problems, expressed in an L^2 basis, appeared, several algorithms were suggested to accelerate the convergence of the results within a restricted subset of the basis. For instance, Heller and Yamani [8] used ''Kato correction,'' and Sotona, Revai, and Zofka [9] introduced the ''Lanczos factor.'' A more intuitive approximation was proposed by Vasilevsky, Filippov, and Chopovsky [6].

The analysis of the AM equations presented in this work will be shown to lead to (1) an optimal choice for the basis, given the potential, yielding well converging and stable solutions of the AM system, or, if the optimal basis cannot be used, to (2) algorithmic procedures for solving the AM system in an acceptable and controlled approximation. These algorithmic procedures will depend on the specific choice made for the basis (i.e., the oscillator radius chosen), but also on information on the asymptotic behavior of the expansion coefficients, as well as on the dynamical equations themselves. In this way the algorithm used will depend on the physical properties of the system considered. In a forthcom-

ing paper the different strategies for solving AM equations will be applied explicitly to a number of problems from nuclear, atomic, and molecular physics.

II. THE AM IN AN OSCILLATOR BASIS

Choosing an oscillator basis to describe some specific Hilbert subspace in which to solve the Schrödinger equation leads to the following form of the latter in terms of a system of linear equations:

$$\sum_{m=0}^{\infty} \langle n|\hat{H}-E|m\rangle c_m = 0, \tag{1}$$

where the coefficients c_m are the expansion coefficients in the oscillator basis of the wave function corresponding to the energy E

$$|\Psi_E\rangle = \sum_{n=0}^{\infty} c_n |n\rangle, \tag{2}$$

and subject to a typical boundary condition. For simplicity we have omitted the angular momentum quantum number as well as the energy dependence of the coefficients c_n.

The boundary conditions of quantum systems are traditionally expressed in coordinate space, but can also be formulated in terms of the expansion coefficients c_n. Indeed, for very large n, the dynamical equations are reduced to a simple (in an oscillator basis a three-term recurrence) form containing the kinetic-energy operator solely. The equations can therefore be solved analytically for very large n [2,4,5]. The above mentioned reduction of the equations only involves the supposition that the potential energy matrix elements vanish for very large n, which has been shown to be an acceptable approximation for relatively short-range interactions.

One obtains the following asymptotic behavior for bound states:

$$c_n^{(as)} \simeq \sqrt{R_n}\exp(-\kappa R_n)/R_n, \tag{3}$$

$$(\kappa = \sqrt{-2mE/\hbar^2})$$

and for continuum states:

$$c_n^{(as)} \simeq \sqrt{R_n}[j_L(kR_n) + \tan(\delta) n_L(kR_n)], \tag{4}$$

$$(k = \sqrt{2mE/\hbar^2})$$

where j_L and n_L are the traditional Bessel and Neumann special functions.

A striking resemblance with the asymptotic forms of a wave function in coordinate representation is observed, by replacing the radial coordinate in the latter by the discrete value $R_n = \sqrt{4n+2L+3}$. A heuristic argument for this observation is that R_n corresponds to the turning point of the oscillator in state $|n\rangle$ with angular momentum L.

III. A SIMPLE SCHEME FOR SOLVING THE AM SYSTEM OF EQUATIONS

In the preceding section we introduced the infinite dimensional system of linear equations obtained from the AM formulation, to be solved subject to a proper boundary condition. As indicated earlier we will concentrate on the scattering situation, and therefore only consider the asymptotic behavior of the c_n corresponding to the continuum boundary condition.

A scheme for solving the linear system of equations quite naturally presents itself. Under the assumption that the matrix elements potential energy $\langle i|V|j\rangle$ vanish for sufficiently large values of one of the basis state indices i or j, one chooses a limiting value N to set this vanishing point in terms of the basis states. In the region where the potential matrix elements are neglected, the expansion coefficients c_n are then given by (4), and can be written as

$$c_n = c_n^{(+)} + \tan(\delta) c_n^{(-)} \quad (n \geqslant N) \tag{5}$$

assuming N to be sufficiently large, with

$$c_n^{(+)} = \sqrt{R_n} j_L(kR_n) \quad (n \geqslant N)$$

$$c_n^{(-)} = \sqrt{R_n} n_L(kR_n) \quad (n \geqslant N). \tag{6}$$

The choice for N divides the linear system in three different regions:

(i) a finite number of N equations with $0 < n < N$, in which the potential energy matrix elements are fully taken into account. These equations correspond to the ''internal region'' in terms of the basis states.

(ii) an infinite number of equations corresponding to $n > N$, in which the potential energy matrix elements are neglected. These equations correspond to the ''asymptotic region,'' and are trivially fulfilled due to the boundary condition.

(iii) the equation with $n = N$, in which the potential matrix elements are neglected. This equation corresponds to the ''matching condition,'' as it couples the internal region through coefficient c_{N-1} with the asymptotic region through the phase shift δ.

This scheme amounts to solving the following $N+1$ dimensional system of linear equations for the N coefficients c_n with $n = 0,1,\ldots,N-1$, and the phase shift δ:

$$\begin{pmatrix} H_{00}-E & \cdots & H_{0,N-1} & 0 \\ \vdots & \vdots & \vdots & \vdots \\ H_{N-1,0} & \cdots & H_{N-1,N-1}-E & T_{N-1,N} c_N^{(-)} \\ 0 & \cdots & T_{N,N-1} & \mathcal{T}_N^{(-)} \end{pmatrix} \begin{pmatrix} c_0 \\ \vdots \\ c_{N-1} \\ \tan(\delta) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ -T_{N-1,N} c_N^{(+)} \\ -\mathcal{T}_N^{(+)} \end{pmatrix}, \tag{7}$$

where

$$\mathcal{T}_N^{(+)}=(T_{N,N}-E)c_N^{(+)}+T_{N,N+1}c_{N+1}^{(+)}$$

$$\mathcal{T}_N^{(-)}=(T_{N,N}-E)c_N^{(-)}+T_{N,N+1}c_{N+1}^{(-)} \tag{8}$$

and T stands for the kinetic-energy operator.

As the potential matrix elements do not actually drop to zero exactly for $n \geqslant N$, one should vary the value of N to test the stability of the solution. It turns out that this stability strongly depends on the specific problem considered. As an example, the solution of the linear system of equations for a nuclear two-cluster problem, in which the distance of the clusters is considered as the degree of freedom, shows a rapid convergence in terms of N. A solution for a monopole description of the nucleus, in which the radius of the nucleus is considered to be the prominent degree of freedom, shows a very slow convergence in terms of N. These results indicate that one should be very careful when omitting potential energy matrix elements, and that a proper study of the form of the equations is necessary.

IV. AN ANALYSIS OF THE AM EQUATIONS

A. A reformulation of the AM equations

To study the properties of the (in principle infinite dimensional) linear system (1) to be solved, we will rewrite this set of equations using the following substitution for the expansion coefficients c_n:

$$c_n=c_n^{(as)}+c_n^{(0)}. \tag{9}$$

By this substitution, the coefficients c_n are considered to represent a deviation from the asymptotic behavior, i.e., the coefficients $c_n^{(as)}$. The coefficient $c_n^{(0)}$ then quantifies this deviation, which, in particular, will be zero in the true asymptotic region (i.e., for very large n). The first term in (9) is responsible for the long-range behavior of the system. The second term corresponds to the short-range correction caused by the potential; in other words, in coordinate representation the coefficients $\{c_n^{(0)}\}$ would represent that part of the wave function that is dominated by, and within the range of, the potential. The knowledge of $c_n^{(0)}$ as a function of n thus provides a key element for determining a proper index N distinguishing the internal from the asymptotic region in terms of the basis functions.

Rewriting the original AM linear system of equations (1) in the unknowns $(\{c_n\})$, yields an equivalent linear system in the unknowns $(\{c_n^{(0)}\},\delta)$, where δ is defined by the following form of the asymptotic expansion coefficients $c_n^{(as)}$:

$$c_n^{(as)}=c_n^{(+)}+\tan(\delta)c_n^{(-)}. \tag{10}$$

Because the asymptotic coefficients now appear for all n in this representation, they should be properly defined. In order to do so, we consider the coordinate representation of the outgoing asymptotic wave functions $\Psi^{(+)}$ and $\Psi^{(-)}$, which are originally defined as the two linearly independent solutions of

$$(\hat{T}-E)\Psi=0, \tag{11}$$

where $\hat{T}$ is the kinetic-energy operator. $\Psi^{(+)}$ is commonly called the ''regular'' solution, and behaves properly for all r. $\Psi^{(-)}$ is the ''irregular'' solution, and has an irregular (infinite) behavior near the origin $r=0$. To provide a regular character at the origin for both $\Psi^{(+)}$ and $\Psi^{(-)}$, we redefine their equations in the following way, as was suggested earlier by Heller and Yamani [1]:

$$(\hat{T}-E)\Psi^{(+)}=0,$$

$$(\hat{T}-E)\Psi^{(-)}=\beta_0\Phi_0. \tag{12}$$

The nonzero right-hand side in (12), in which $\Phi_0(r)=\langle r|0\rangle$ represents the zero-quanta oscillator state, and where β_0 equals

$$\beta_0=\hbar\omega\frac{\exp(k^2/2)}{k^{L+1}}\left[\frac{2}{\Gamma(L+1/2)}\right]^{1/2}\frac{1}{\Gamma(-L+1/2)} \tag{13}$$

accounts for a regular behavior near the origin for the modified $\Psi^{(-)}$

$$\Psi^{(-)}(kr)\approx\begin{cases} j_L(kr) & \text{for } r\ll 1 \\ n_L(kr) & \text{for } r\gg 1 \end{cases}. \tag{14}$$

In terms of a Fourier representation, using oscillator states as a basis, one then has the following well-defined expansion:

$$\Psi^{(+)}(r)=\sum_{m=0}^{\infty}\langle r|m\rangle c_m^{(+)},$$

$$\Psi^{(-)}(r)=\sum_{m=0}^{\infty}\langle r|m\rangle c_m^{(-)}. \tag{15}$$

This provides a proper definition for the coefficients $c_n^{(+)}$ and $c_n^{(-)}$ in (10), the ''regular,'' respectively, ''irregular'' asymptotic coefficients, the explicit form of which can be found in [2,5]. The equations for the asymptotic coefficients in Fourier space are then

$$\sum_{m=0}^{\infty}\langle n|\hat{T}-E|m\rangle c_m^{(+)}=0,$$

$$\sum_{m=0}^{\infty}\langle n|\hat{T}-E|m\rangle c_m^{(-)}=\beta_0\delta_{n,0}. \tag{16}$$

One notices an identical form for all equations, except for the single one with $n=0$.

Substituting the solutions of (16) for the asymptotic coefficients in the set of equations (1), taking into account the substitutions (9) and (10), then leads to the following linear system:

$$\sum_{m=0}^{\infty}\langle n|\hat{H}-E|m\rangle c_m^{(0)}+\tan(\delta)\left[\beta_0\delta_{n,0}+\sum_{m=0}^{\infty}\langle n|\hat{V}|m\rangle c_m^{(-)}\right]$$

$$=-\sum_{m=0}^{\infty}\langle n|\hat{V}|m\rangle c_m^{(+)}. \tag{17}$$

Equation (17) now shows the influence of the potential-energy matrix elements on the behavior of the system in a clear way.

Let us introduce the ''dynamical regular and irregular coefficients'' $V_n^{(+)}$ and $V_n^{(-)}$ as follows:

$$V_n^{(+)}=\sum_{m=0}^{\infty}\langle n|\hat{V}|m\rangle c_m^{(+)}$$

$$V_n^{(-)}=\sum_{m=0}^{\infty}\langle n|\hat{V}|m\rangle c_m^{(-)} \tag{18}$$

or, in an alternative integral representation in three-dimensional coordinate space

$$V_n^{(+)}=\int_0^{\infty} dr\, r^2\Phi_n(r)\hat{V}(r)\Psi^{(+)}(kr),$$

$$V_n^{(-)}=\int_0^{\infty} dr\, r^2\Phi_n(r)\hat{V}(r)\Psi^{(-)}(kr), \tag{19}$$

where we use the coordinate representation of $\Phi_n(r)$, the n-quanta oscillator function $\langle r|n\rangle$

$$\Phi_n(r)=(-1)^n N_{nL}\rho^L\exp(-\tfrac{1}{2}\rho^2)L_n^{L+(1/2)}(\rho^2)\quad\left(\rho=\frac{r}{b}\right),$$

$$\left\{N_{nL}=\left[\frac{2(n!)}{\Gamma(n+L+3/2)}\,\frac{1}{b^{3/2}}\right]^{1/2}\right\}. \tag{20}$$

Substitution of the dynamical coefficients (18) in (17) leads to

$$\sum_{m=0}^{\infty}\langle n|\hat{H}-E|m\rangle c_m^{(0)}+\tan(\delta)[\beta_0\delta_{n,0}+V_n^{(-)}]=-V_n^{(+)}. \tag{21}$$

No approximations have been made so far to obtain this representation of the AM dynamical equations. We have taken into account the main (asymptotic) behavior of the solutions in the equations, and used a regularization scheme to achieve this in a well-defined way.

To reveal how the AM linear system can be solved in a numerically optimal, or at least acceptable, way, an analysis of the dynamical coefficients $V_n^{(+)}$ and $V_n^{(-)}$ seems imperative. It is indeed clear that, if, e.g., $V_n^{(+)}$ and $V_n^{(-)}$, from a given index n on, are sufficiently zero when compared to the other terms in (21), the equations are reduced in a controlled and secure way.

There is another important reason to investigate the behavior of $V_n^{(+)}$. It is indeed well known from the integral equation formulation of quantum mechanics [10] that

$$\tan\delta_L=-\frac{mk}{\hbar^2}\int_0^{\infty} dr\,\Psi^{(+)}(kr)\hat{V}(r)\Psi(k,r), \tag{22}$$

where $\Psi(k,r)$ is the exact solution of the Schrödinger equation obtained with potential $\hat{V}$. In an oscillator representation, (22) reads as

$$\tan\delta_L=-\frac{mk}{\hbar^2}\sum_{n=0}^{\infty} V_n^{(+)}c_n \tag{23}$$

from which we immediately recognize the importance of $V_n^{(+)}$ in the convergence of the solutions of the continuous spectrum.

The analysis of $V_n^{(+)}$, $V_n^{(-)}$ must be done in terms of the basis index n, of the oscillator parameter b fixing the basis, and of the potential-energy parameters. Results emerging from such an analysis can then be checked by studying the solutions $c_n^{(0)}$ and $\tan(\delta)$ as a function of the same parameters.

B. A model analysis using the Gaussian potential

To analyze the behavior of the AM set of linear equations and its defining quantities in a more or less general way, we consider a simple Gaussian potential of the form

$$\hat{V}(r)=V_0\exp\left[-\left(\frac{r}{a}\right)^2\right]. \tag{24}$$

There are a number of reasons to justify such a choice: (1) an operator with Gaussian functional form is easily handled in a harmonic-oscillator basis, as matrix elements can be calculated using closed expressions, or simple recurrence formulas; (2) (semi-) realistic potentials are often expressed explicitly as a finite sum of Gaussians, each with specific amplitude and width parameters, and are of common use, e.g., in nuclear physics calculations; (3) a very large class of potentials can be expressed in terms of a Gaussian transform, such as, e.g., a Yukawa or a Coulomb potential.

In general the matrix elements of the potential-energy operator, due to the r/a dependence of the latter, will depend on the ratio b/a. In the specific case of a Gaussian potential one has an explicit dependence on

$$\gamma=\left(\frac{b}{a}\right)^2. \tag{25}$$

This means that matrix elements of the Gaussian-potential-energy operator in an oscillator basis are invariant under all scale transformations of a and b which preserve γ, and different physical situations will lead to the same matrix $\langle n|\hat{V}|m\rangle$. In particular, small values of γ are realized by small values of b relative to a, or large values of a relative to b; this situation corresponds to a ''long-range'' potential. Large values of γ correspond likewise to a ''short-range'' potential.

The potential is certainly not the only parametrized quantity characterizing the set of AM equations. The oscillator radius of the oscillator basis is another and equally important parameter, because of the repercussion on the values of both the kinetic and potential matrix elements appearing in the equations. In this section we will therefore study the behavior of the AM equations as a function of both the oscillator radius of the basis, and the width of the Gaussian potential. Actually, as indicated by (25) only the ratio of these quantities is required, without any loss of generality for the current analysis. We therefore make a specific choice of potential parameters, namely $V_0=-8$ MeV and $a=1$ fm, so that the

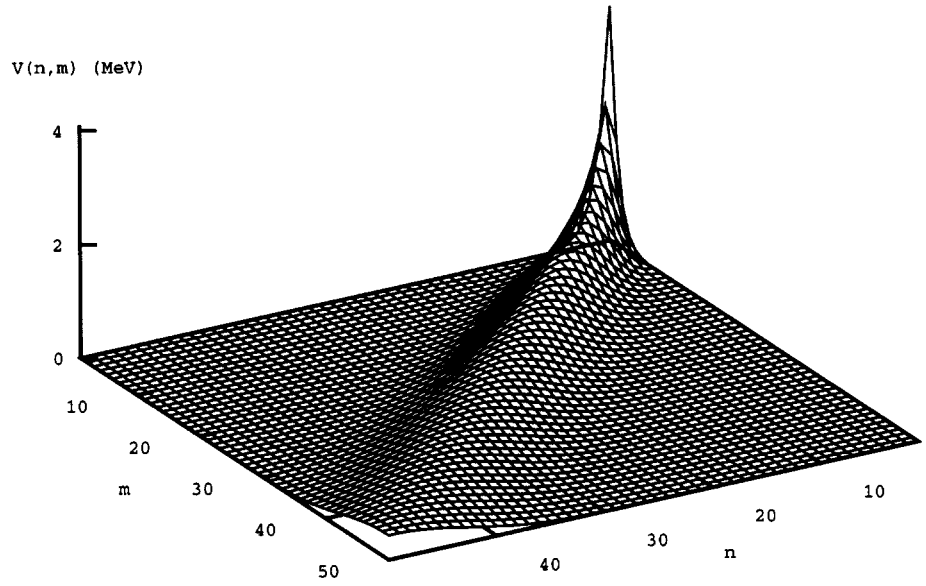

FIG. 1. Matrix elements of a Gaussian potential in an oscillator basis with width parameter $b=0.75$. The horizontal axes are labeled by the basis index, the vertical axis is in MeV.

potential has both a discrete and continuous spectrum. The γ ratio will then be varied by adapting the oscillator radius b.

A central theme in the analysis is the characterization for a rapidly converging, and stabilized, solution of the AM equations. This is most naturally done by searching for a maximal, limiting, value for the number of basis states involved in a specific solution, depending on the problem parameters used. As the asymptotic behavior of the solution is governed essentially by the kinetic-energy term, one should therefore take into account how both potential and kinetic matrix elements behave with respect to one another. In other words, it is not sufficient to know about the insignificance of potential matrix elements in absolute terms to decide whether one has reached the asymptotic region, but rather consider some relative insignificance with respect to the value of the kinetic matrix elements.

When working in a coordinate representation, one can obtain a lot of information concerning the wave function by analyzing the Hamiltonian only, and this both in terms of coordinate and energy ranges. The main reason for this is that the Hamiltonian is globally defined in the whole coordinate space. In a L^2 representation, in our case using an oscillator basis, this is not such a straightforward matter. The main parameters determining the rate of convergence, as well as the behavior of the solution (the wave function in an oscillator representation), are of a ''global'' nature, such as $\Sigma_m\langle n|\hat{V}|m\rangle c_m=\langle n|\hat{V}|\Psi\rangle$, $\langle n|\hat{V}|\Psi^{(+)}\rangle$ and so on. The matrix elements of the kinetic, respectively, potential-energy operators are ''local'' quantities (i.e., the value of these operators in a single point in coordinate space). The study of these elements, however, reveals the peculiarities of the ''global'' quantities, and will help to understand their behavior.

Concerning the kinetic-energy term, two remarks are very important in the context of an oscillator basis. The kinetic-energy contribution has a very simple representation in terms of the oscillator basis: (1) it is proportional to the inverse square of the oscillator radius b, and (2) the kinetic-energy matrix has a tridiagonal form, i.e., has nonzero matrix elements only along the major diagonal and the first subdiagonals.

1. Analysis of the Hamiltonian matrix elements

Figure 1 displays the overall (qualitative) behavior of a typical Gaussian potential matrix in some specific oscillator basis. The main properties to be noted are the comportment of (1) the main diagonal which falls off monotonically for large n, and of (2) the nondiagonal matrix elements with nonzero values concentrated symmetrically around the main diagonal. This structure of the potential contribution is certainly of a promising nature, regarding the earlier remarks concerning the kinetic-energy contribution.

A more quantitative view of the diagonal behavior of the potential matrix is displayed in Fig. 2, and this for a number of choices of oscillator bases. Three different views are presented in this figure: (a) the pure diagonal matrix elements; (b) the diagonal matrix elements multiplied by the square of the oscillator radius (eliminating the kinetic-energy dependence on the choice of basis), and (c) the diagonal matrix elements normalized with respect to the first one; both Figs. 2(a) and 2(b) lead to Fig. 2(c) through this normalization. From these figures it should be clear that one has to be careful when drawing conclusions for a proper choice of basis. Figure 2(a) might suggest that very large values of the oscillator radius b are optimal. Figure 2(b) on the contrary might suggest that very small values of b are optimal. The normalized Fig. 2(c) finally suggests that, for the current potential parameters, the interval for b between 0.25 fm and 2.0 fm would be optimal. Figure 2 at least reveals that there are important differences in behavior of the potential energy contribution for different choices of the oscillator radius. Later on it will be shown in a more quantitative way that the qualitative conclusion for an optimal b interval as suggested

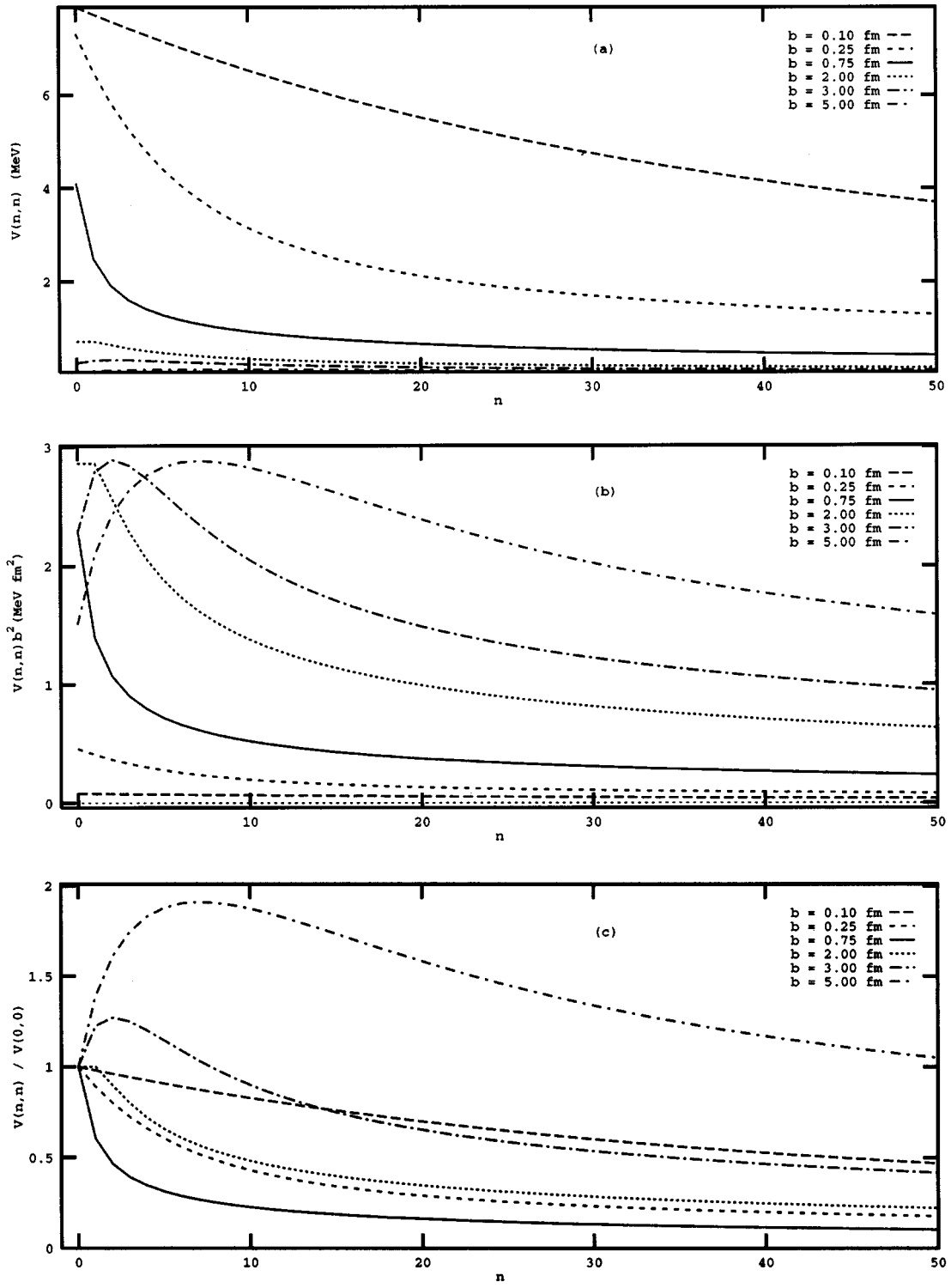

FIG. 2. Diagonal matrix elements of a Gaussian potential in oscillator bases with different width parameter b: (a) exact values in MeV, (b) values weighted with b^2 in Mev fm^2, and (c) values relative to $\langle 0|\hat{V}|0\rangle$. The horizontal axis labels the basis index.

by Fig. 2(c) is correct. An interesting conclusion that is apparent from the figure is that a (coordinate space defined) short-range potential turns out to have a long-range character in an oscillator representation. As the oscillator basis is used as a Fourier basis to portray the solution, this is a well-known effect in terms of Fourier representation theory.

A quantitative view of the nondiagonal behaviour of the potential matrix for the same bases displayed in Fig. 2 can be found in Fig. 3, and this by showing a typical row for a fixed column index ($n=50$ in this case). The same three views (pure, multiplied by b^2, and normalized with respect to the diagonal matrix element with $n=50$) are shown, respectively, in Figs. 3(a), 3(b), and 3(c). Again a strong dependence on the choice of the oscillator radius is remarked, but it is much more difficult to draw conclusions for an optimally converging basis from these figures. As this figure

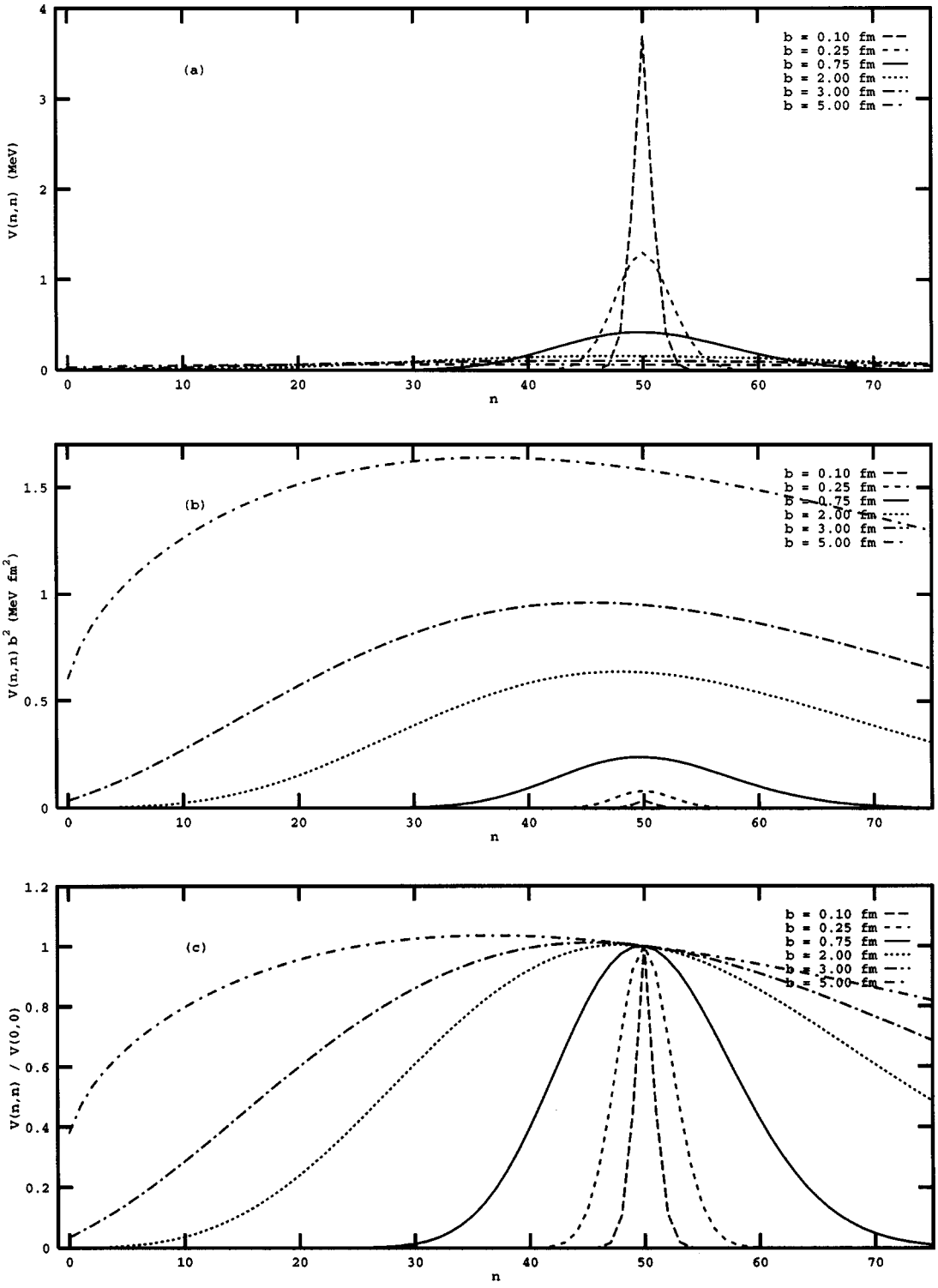

FIG. 3. Matrix elements of a Gaussian potential in oscillator bases with different width parameter b for row index $n=50$: (a) exact values in MeV, (b) values weighted with b^2 in MeV fm^2, and (c) values relative to $\langle 50|\hat{V}|50\rangle$. The horizontal axis labels the (column) basis index.

indicates that the potential-energy contribution is concentrated around the main diagonal of the matrix, but with a relatively important distribution, it should already warn against carelessly applying the simple but straightforward solution scheme presented in Sec. II of this paper!

The previous figures thus only allow us to initiate some general discussion, but not to draw final and well-formed conclusions on the convergence problem, let alone on the determination of an optimal basis and the number of states involved in a stable solution.

2. Analysis of the dynamical coefficients

Up to now only local views of the potential contribution, i.e., matrix elements and their behavior, have been considered to provide possible hints for a properly converging so-

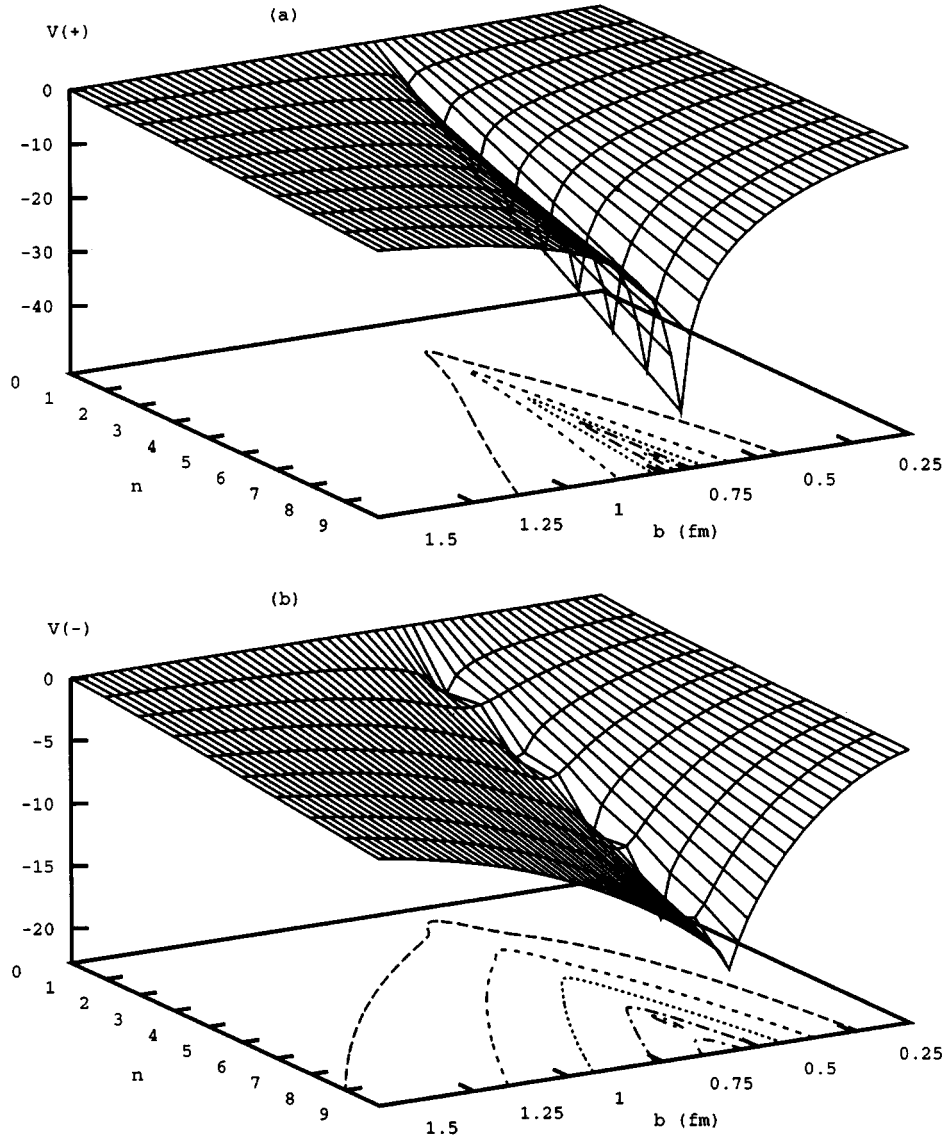

FIG. 4. The dynamical coefficients $|V_n^{(+)}/V_0^{(+)}|$ (a, top) and $|V_n^{(-)}/V_0^{(-)}|$ (b, bottom) as a function of b and n, for an energy of 1 MeV. The vertical axis is logarithmic.

lution. The new representation of the AM equations presented earlier in this section introduced some global quantities which might be of interest in the convergence analysis. These are the dynamical coefficients $V_n^{(+)}$ and $V_n^{(-)}$, and they combine all matrix elements of row n as indicated above. If, and when, these quantities would be (sufficiently) zero from a given value N on, this would certainly determine the maximal number of oscillator states to be considered for a converging solution. As $V_n^{(+)}$ and $V_n^{(-)}$ depend on both the potential and the basis parameters, they will be analyzed as a function of the ratio of potential width to oscillator radius. As $V_n^{(+)}$ and $V_n^{(-)}$ also depend explicitly on energy, this will be an additional parameter to consider.

A qualitative view of $V_n^{(+)}$ is shown in Fig. 4(a) as a function of both the index n and the ratio b/a; the quantity was normalized with respect to $V_0^{(+)}$, and the scale is a logarithmic one. From this figure one immediately notices that a well-defined value of the ratio of the potential to oscillator radius zeroes the quantities for already very small values of n. Figure 4(b) depicts the same view for $V_n^{(-)}$, carrying an analogous conclusion. Although both optimal values do not coincide completely, they are sufficiently close to define a narrow interval of optimal values for a swiftly converging solution. Indeed, if we consider a value N for which $|V_N^{(+)}/V_0^{(+)}|<\epsilon$ and $|V_N^{(-)}/V_0^{(-)}|<\epsilon$ (with, e.g., $\epsilon<10^{-6}$), we can assume to have reached the asymptotic region. The value N then determines the number of basis functions needed to obtain a well-converged solution. Indeed, the solutions of (17) are deviations with respect to the (known) asymptotic solutions, and become zero when both $V_n^{(+)}$ and $V_n^{(-)}$ are (sufficiently) zero. In other words, the value N from which on $V_n^{(+)}$ and $V_n^{(-)}$, and thus the solutions $c_n^{(0)}$, are zero determines what would be called in the resonating group method (RGM) terminology the matching point between the internal and the asymptotic region. It is important to remark that N is determined prior to solving the AM equa-

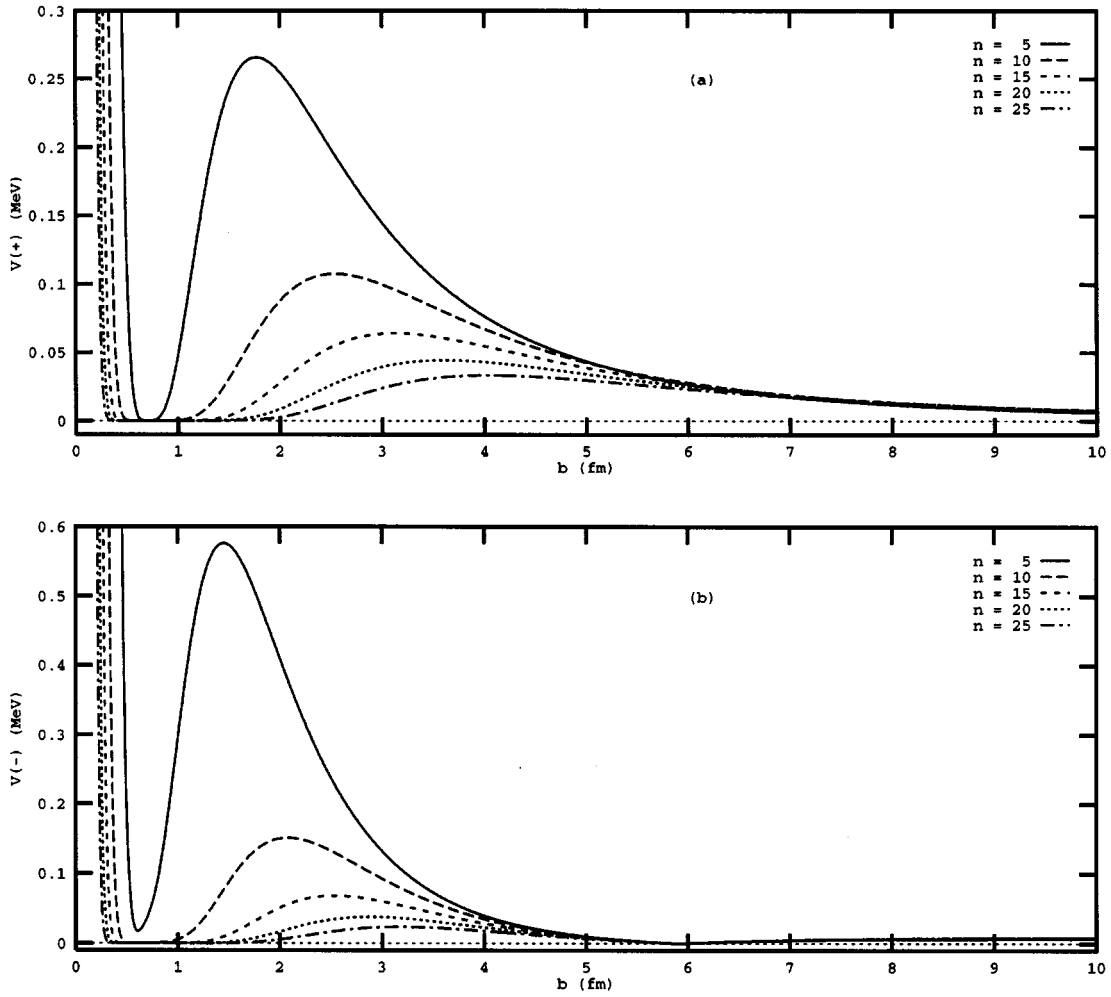

FIG. 5. $V_n^{(+)}$ (a, top) and $V_n^{(-)}$ (b, bottom) as a function of b for various values of n and an energy of 1 MeV.

tions, and is obtained from the simple knowledge of the potential-energy matrix elements.

To corroborate the fact for an optimal choice of basis for a given Gaussian potential, a quantitative view of $V_n^{(+)}$ and $V_n^{(-)}$ as a function of the radius parameter b is shown in Figs. 5(a) and 5(b) for a selected number of n values. From this figure one can determine for which values of the radius parameter one obtains a properly converged solution, by considering the intersection of both optimal intervals for $V_n^{(+)}$ and $V_n^{(-)}$. One notices that for a potential consisting of a single Gaussian term, a very limited number of basis states is necessary for a proper convergence. For more intricate potential forms this will not necessarily be the case, although an optimal value for the radius parameter, be it associated with a relatively larger value of N, will still be available.

To check the dependence of the so-called ''optimal'' b values (or regions) as a function of energy, Fig. 6 displays the values of both $V_n^{(+)}$ and $V_n^{(-)}$, relative to, respectively, $V_0^{(+)}$ and $V_0^{(-)}$ for varying b and energy for a fixed n. It is important to notice that, at least for the Gaussian potential, the optimal value for the oscillator radius is independent of energy.

Finally Fig. 7 shows the quantitative behavior of $V_n^{(+)}$ and $V_n^{(-)}$, again relative to, respectively, $V_0^{(+)}$ and $V_0^{(-)}$, as a function of n. From these figures one easily obtains an optimal number of basis functions, given the specific parameters of the problem and the precision considered. As a hands on example, Fig. 7 indicates that, for a precision of about 10^{-8}, less than 12 basis functions are needed for all b values between 0.5 fm and 1 fm.

The conclusions above indicate the importance of the $V_n^{(+)}$ and $V_n^{(-)}$ quantities, and a closer investigation imposes itself. A closed expression for $V_n^{(+)}$ can be obtained in a straightforward way as

$$V_n^{(+)} = V_0 \frac{(1-2\gamma)^n}{(1+2\gamma)^{n+L+3/2}} k^L \times \exp\left(-\frac{1}{2}k^2 \frac{1}{1+2\gamma}\right) N_{nL} L_n^{L+1/2}\left(\frac{k^2}{1-4\gamma^2}\right) \qquad (26)$$

for which the full calculation is reproduced in the Appendix.

This expression features a single minimum in terms of γ, namely, for $\gamma = 1/2$ or $b = a/\sqrt{2}$, with a value

$$V_n^{(+)} = V_0 N_{nL} \frac{1}{4} \frac{1}{n!} \left(\frac{k}{2}\right)^{2n+L+1/2} \exp\left(-\frac{1}{4}k^2\right), \qquad (27)$$

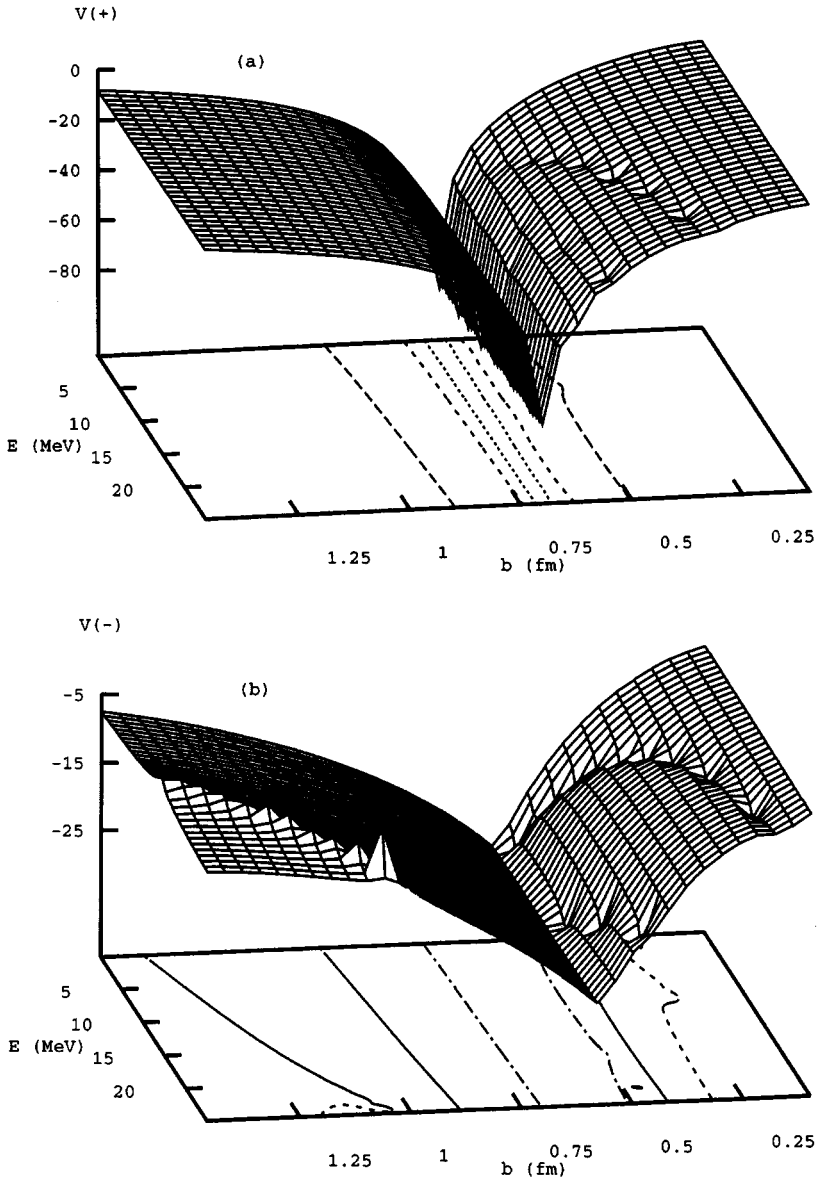

FIG. 6. $|V_n^{(+)}/V_0^{(+)}|$ (a, top) and $|V_n^{(-)}/V_0^{(-)}|$ (b, bottom) as a function of b and E, for $n=20$. E values are in MeV and the vertical axis is logarithmic.

which drops off to zero very fast in terms of n because of its following behavior:

$$V_n^{(+)} \approx \frac{1}{n! R_n^{L+1/2}}. \tag{28}$$

Both position and behavior of $V_n^{(+)}$ around this minimum were already apparent from the foregoing figures.

The asymptotic behaviour of $V_n^{(+)}$ for both small and large values of γ is also readily obtained. For small values of γ (i.e., small values of the oscillator radius b compared to the potential width a) Eq. (26) yields the following asymptotic form, valid for large n:

$$\begin{aligned} V_n^{(+)} &\approx V_0 \exp\{-\gamma R_n^2\} c_n^{(+)} \\ &\approx V_0 \exp\{-\gamma R_n^2\} \sqrt{2R_n} j_L(kbR_n). \end{aligned} \tag{29}$$

This expression consists of two factors in coordinate representation, the Gaussian potential $\hat{V}(r)$ and the (asymptotic) wave function $\Psi^{(+)}(k,r)$, both evaluated in one and the same discrete point $r=bR_n$ [R_n is the classical turning point, cf. (3) and (4)]. For γ approaching zero the expression shows a slowly decreasing behavior of $V_n^{(+)}$ as a function of n.

For large values of γ one obtains the following asymptotic form valid for large n:

$$V_n^{(+)} \approx (-1)^n V_0 \frac{1}{2\gamma} \left(\frac{2}{k}\right)^{1/2} \exp\left\{-\frac{R_n^2+k^2}{4\gamma}\right\} I_{L+1/2}\left(\frac{k}{2\gamma} R_n\right), \tag{30}$$

which for the limiting case of γ now approaching infinity again displays a slowly decreasing behavior as a function of n.

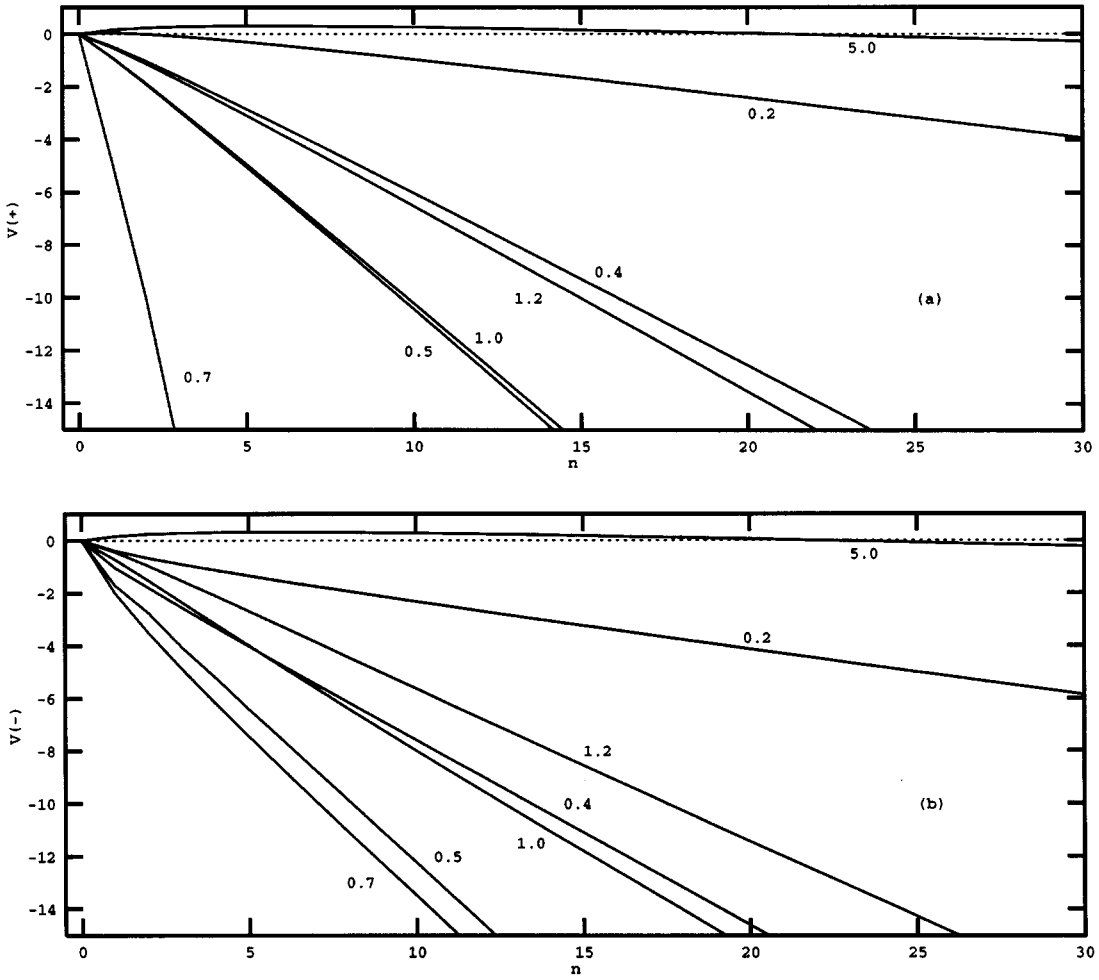

FIG. 7. Logarithmic plot of $|V_n^{(+)}/V_0^{(+)}|$ (a, top) and $|V_n^{(-)}/V_0^{(-)}|$ (b, bottom) as a function of n for several values of the oscillator radius b and an energy of 1 MeV. The vertical axis shows orders of magnitude.

Both very large and very small values of γ will thus lead to rather badly converging solutions, which essentially means that a large number of basis functions will have to be considered when γ reaches towards limiting values. This discussion on asymptotic behavior confirms conclusions already apparent from the numerically calculated figures of $V_n^{(+)}$.

Figure 8 indicates that the asymptotic formulas are quite valid for a broad range of b values, and as such, can often be used to obtain reasonable values for N for properly converged solutions. Indeed, as the main factor which defines the decreasing behavior of $V_n^{(+)}$ for small, respectively, large values of γ, is the potential term, which has the value $\exp\{-\gamma R_n^2\}$, respectively, $\exp\{-(R_n^2/4\gamma)\}$, as can be seen in Eqs. (29) and (30). So, if one considers, e.g., 10^{-6} to be a reasonable measure for precision, one can write approximately

$$\left|\frac{V_n^{(+)}}{V_0^{(+)}}\right| \approx \begin{cases} \exp\{-\gamma R_n^2\} = 10^{-6} & (\text{small}\,\gamma) \\ \exp\left\{-\dfrac{R_n^2}{4\gamma}\right\} = 10^{-6} & (\text{large}\,\gamma), \end{cases} \tag{31}$$

which immediately leads to the respective values $N \approx 14/(4\gamma)$ (for small γ) and $N \approx 14\gamma$) (for large γ); for a value of $b/a = 0.2$ one obtains $N \approx 90$, and for $b/a = 3.0$ $N \approx 125$.

The asymptotic behavior of $V_N^{(+)}$ can be used to an even better extent, by taking it into account when solving the AM system of equations. This will be pursued in full detail in a forthcoming section. Although more intricate to develop, an analogous analysis can be made for $V_n^{(-)}$, leading to corresponding conclusions.

3. Analysis of the phase shifts

In Fig. 9 we show the phase shifts obtained at an energy of $E = 1$ MeV for different values of γ (actually in all further results $a = 1.0$ fm, so that b and γ coincide), as a function of the number of basis states involved in the calculation. One notices an important gain in convergence speed (and thus precision) when using the reformulated version of the AM equations (21), although small and large b (or γ) values still require an important number of basis states.

On the same figure the normalized $c_n^{(0)}$ solutions are shown for different values of b (γ), for a calculation involving 100 basis states. These results are normalized with respect to the norm W

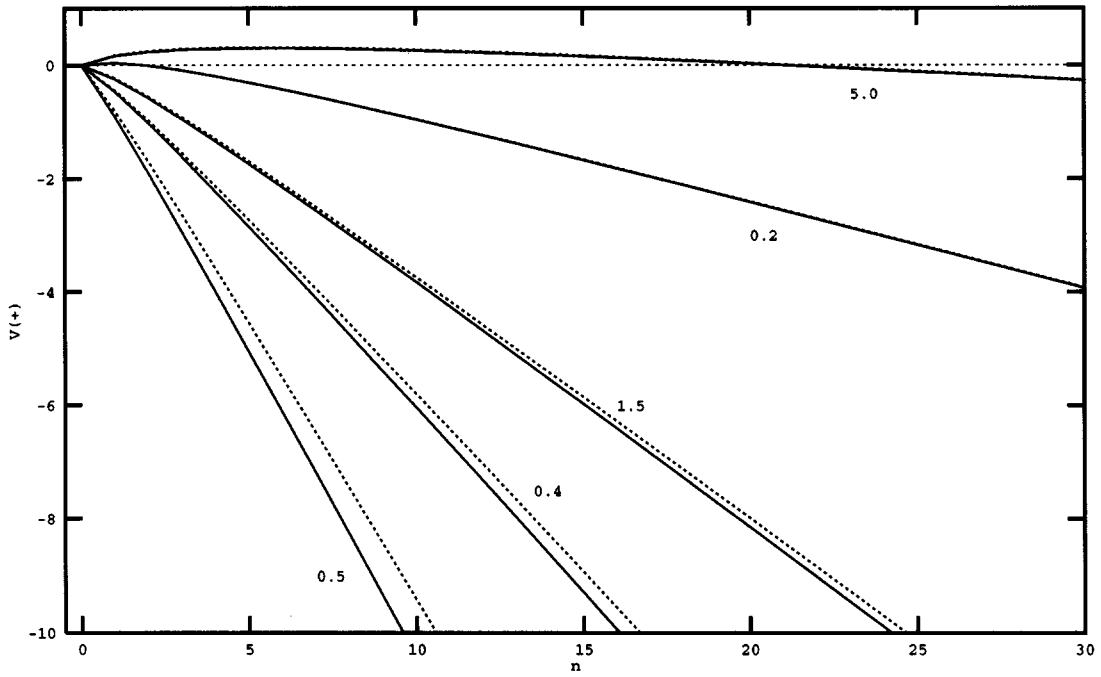

FIG. 8. $|V_n^{(+)}/V_0^{(+)}|$ compared to the asymptotic formulas discussed in the text, as a function of n in a logarithmic plot. The vertical axis shows orders of magnitude.

$$W=\frac{\Sigma_{n=0}^{99}|c_n^{(0)}|^2}{\Sigma_{n=0}^{99}|c_n|^2}, \tag{32}$$

which is also included in the figures. One notices from this value that in the ''optimal b (γ)'' region very few, very small $c_n^{(0)}$ contribute to the solution.

The results displayed on Fig. 9 confirm our suggestion made by analyzing the behavior of $V^{(+)}$ and $V^{(-)}$, i.e., that for optimal values of b (γ) convergence is achieved with less than 12 basis functions. They also confirm that for $b=0.2$ one can use approximately 75, and for $b=3.0$ approximately 100 basis states for reasonable convergence; the latter were indeed overestimated by the numbers obtained from Eq. (31).

To corroborate the fact that the reformulated AM equations (21) provide faster converging solutions, we show in Fig. 10 both the c_n and $c_n^{(0)}$ coefficients obtained in a calculation at $E=1$ MeV and $b=3.0$, with a total number of 100 basis states. This picture confirms the fact that the true solution indeed deviates only by a small amount from the asymptotic one.

To show the dependence of the results on energy, we show in Fig. 11 the phase shift obtained with 5, 10, and 15 basis states compared to the exact results, and this with the original (''simple'') version (7) and the reformulated version (21) of the AM equations. For b values deviating reasonably from the optimal value, the latter form of the equations is seen to be highly superior to the original one. For very small and very large b values, the convergence is still problematic.

V. STABLE SOLUTIONS FOR THE AM EQUATIONS

In the preceding section we obtained interesting results concerning the convergence behavior of the solutions of the AM equations in terms of the parameters defining the basis and the potential energy. It was shown for a Gaussian potential that the rate of convergence was reliably predictable.

The parameter γ or, for fixed potential width a, the oscillator radius b determines the rate of convergence of the expansion $\Psi=\Sigma_n c_n|n\rangle$. It was indeed seen that an optimal value (or a restricted range of optimal values) for b leads to very fast convergence. However, values deviating more or less strongly from the optimal b lead to slowly converging and numerically unprecise results.

As it is not always possible in a realistic calculation to choose the optimal b, for physical as well as for numerical reasons, it is important to develop strategies for stable results even in nonoptimal b regions. This problem was already recognized in [7], were a coupled channels calculated for ^{4}He was performed with the AM, in which both cluster and collective configurations were taken into account: the b value was fixed by physical arguments (essentially optimizing the cluster channel results), and very nonoptimal for the collective channels (in particular, the monopole mode).

The following subsections indicate how such problems can be solved by considering strategies to solve the AM equations, without modifying the original physical problem (e.g., by tampering with b).

A. A general analysis of the asymptotics

We attempt to evaluate the asymptotic behavior (i.e., for $n\gg 1$) for the expansion coefficients $c_n=\langle n|\Psi\rangle$ and the matrix elements $\langle n|\hat{V}|\Psi\rangle$, using only very general information on the (unknown) wave function Ψ. Based on this formulation we will then introduce strategies to overcome the slow-convergence situations. All assumptions made, and results obtained, will be checked against those produced with a Gaussian potential.

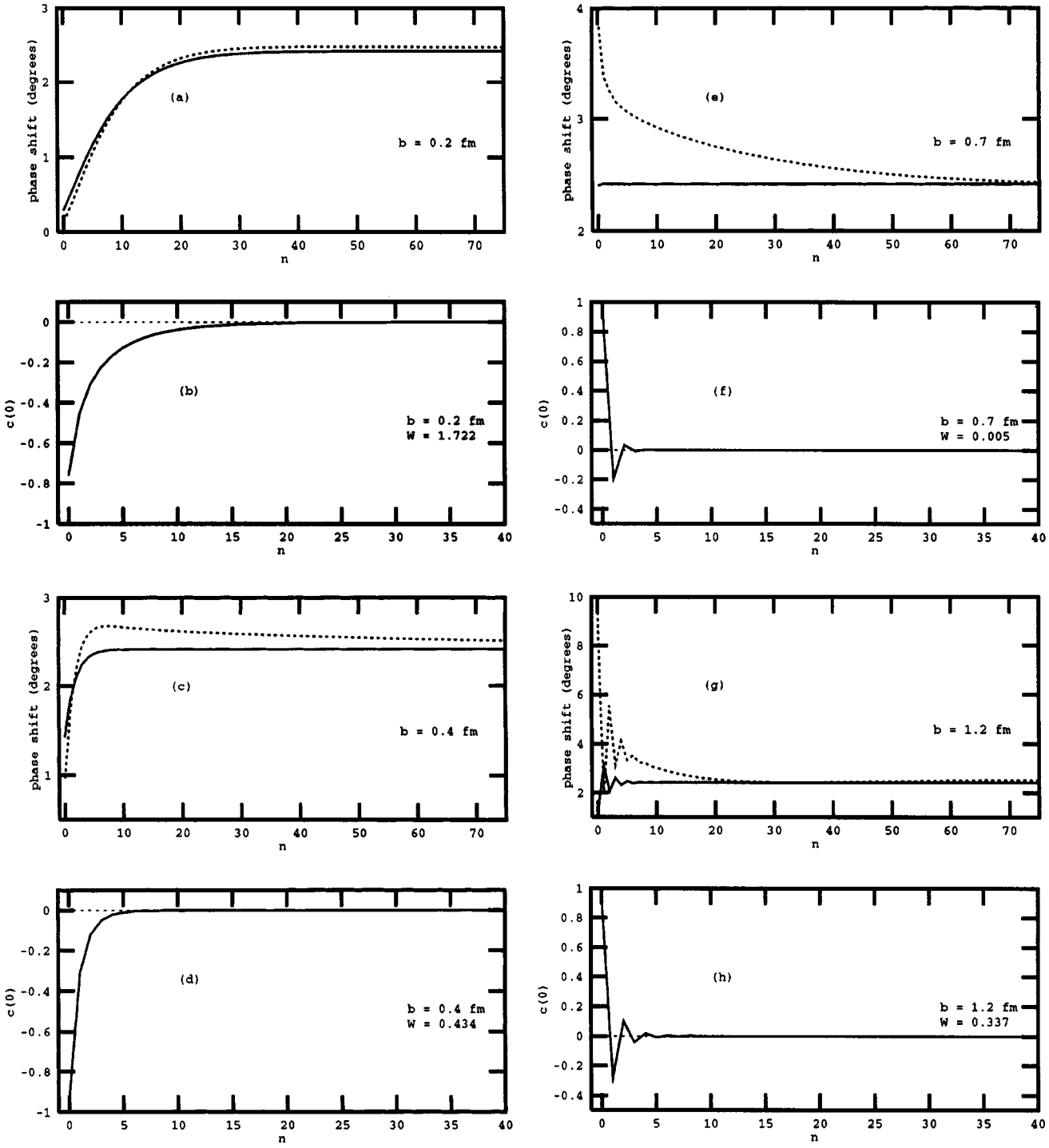

FIG. 9. Left side figures: phase shift δ (degrees) as a function of the number of basis states involved in the calculations; the energy was fixed at 1 MeV. Dotted lines refer to the solutions obtained in the original (''simple'') formulation, full lines refer to solutions obtained in the reformulated version. Right side figures: normalized $c_n^{(0)}$ values (see text) for a calculation with 100 basis states. The norm W is given as a percentage.

To derive a general view on the asymptotic behavior of the Fourier coefficients c_n, we use a generator coordinate (GC) representation for the wave function Ψ

$$\Psi(r)=\int_0^\infty d\beta g(\beta) r^L \exp\{-\beta^2 r^2\} \tag{33}$$

using a scaled Gaussian $\langle r|\beta\rangle = r^L \exp\{-\beta^2 r^2\}$ as a kernel of the integral transformation. It is well known that this kernel provides an alternative, continuous, basis to the traditional, discrete, oscillator basis. A tacit assumption in (33) is that the continuous spectrum wave functions are representable by such a representation, [in particular, that a ''reasonable'' form for $g(\beta)$ exists, leading to an integrable result].

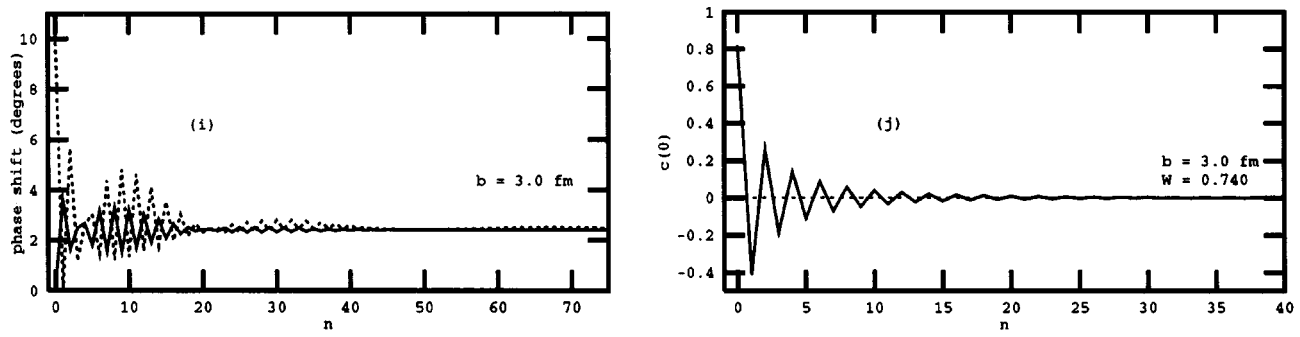

FIG. 9 (*Continued*).

1. Asymptotics of c_n

The Gaussian kernel of (33) is easily expanded in terms of the oscillator basis used throughout this paper. The basis functions $|n\rangle$ are explicited in a coordinate representation by (20).

By substituting ρb for r in the integral kernel $r^L \exp\{-\beta^2 r^2\}$, one can recognize the generating function for the oscillator functions

$$(1+\varepsilon)^{-L-3/2}\rho^L \exp\left\{-\frac{1}{2}\frac{1-\varepsilon}{1+\varepsilon}\rho^2\right\} = \sum_{n=0}^{\infty}\frac{\varepsilon^n}{N_n}|n\rangle, \quad (34)$$

where

$$\beta^2 b^2 = \frac{1}{2}\frac{1-\varepsilon}{1+\varepsilon} \quad \text{or} \quad \varepsilon = \frac{1-2\beta^2 b^2}{1+2\beta^2 b^2}. \quad (35)$$

The expansion coefficients $\langle n|\beta\rangle$ of $\exp\{-\beta^2 r^2\}$ in the oscillator basis are then

$$\langle n|\beta\rangle = (1+\varepsilon)^{L+3/2}\frac{\varepsilon^n}{N_n}b^L = \frac{(1-2\beta^2 b^2)^n}{(1+2\beta^2 b^2)^{n+L+3/2}}\frac{2^{L+3/2}}{N_n}b^L \quad (36)$$

from which one obtains the expansion coefficients $c_n = \langle n|\Psi|\rangle$ of Ψ in the oscillator basis as

$$\langle n|\Psi\rangle = \int_0^\infty d\beta\, g(\beta)\langle n|\beta\rangle = \int_0^\infty d\beta\, g(\beta)\frac{(1-2\beta^2 b^2)^n}{(1+2\beta^2 b^2)^{n+L+3/2}}\frac{2^{L+3/2}}{N_n}. \quad (37)$$

If, and when, $g(\beta)$ is concentrated in a small vicinity of $\beta \approx \beta_0$, one can expect a highly convergent expansion for an oscillator length $b \approx 1/\sqrt{2}\beta_0$.

To study the asymptotic behavior of the expansion coefficients (37), we consider two limiting regions for b, i.e., ''small b'' and ''large b.'' To this end, we rewrite (37) as follows:

$$\langle n|\Psi\rangle = \int_0^{\beta_0} d\beta\, g(\beta)\langle n|\beta\rangle + \int_{\beta_0}^\infty d\beta\, g(\beta)\langle n|\beta\rangle, \quad (38)$$

where $\beta_0 = 1/(\sqrt{2}b)$.

Small b values: for $0 \leqslant \beta < 1/(\sqrt{2}b)$ and large values of n, one can use the following approximate formula:

$$\frac{(1-2\beta^2 b^2)^n}{(1+2\beta^2 b^2)^{n+L+3/2}} \approx \exp\{-R_n^2\beta^2 b^2\}. \quad (39)$$

For large values of n $(n \gg 1)$ one also has

$$\frac{1}{N_n} = \left[\frac{\Gamma(n+L+3/2)}{2\Gamma(n+1)}\right]^{1/2} \approx R_n^{L+1/2}/2^{L+1}, \quad (40)$$

where again R_n is the classical turning point [cf. Eqs. (3) and (4)].

For very small values of b, one can consider only the first term in (38); using the approximations (39) and (40) one then obtains the following asymptotic form of (37):

$$\langle n|\Psi\rangle \approx \sqrt{2}\sqrt{R_n}\int_0^\infty d\beta\, g(\beta)(R_n b)^L \exp\{-R_n^2\beta^2 b^2\}, \quad (41)$$

which, considering (33), leads to the final approximation

$$c_n = \langle n|\Psi\rangle \approx \sqrt{2}\sqrt{R_n}\Psi(bR_n). \quad (42)$$

For small values of the oscillator length b, the expansion coefficients of the wave function $\Psi(r)$ on an oscillator basis are thus proportional to the wave function itself taken at the discrete argument values bR_n.

Such a relationship between the wave function in coordinate space and its oscillator representation was already obtained long ago [4], [1] for the regular and irregular asymptotic solutions. Later, this correspondence has been used as a heuristic principle for solving e.g., the Coulomb problem in an oscillator representation [11].

Large b values: for $1/(\sqrt{2}b) \leqslant \beta < \infty$ and large values of n, one can use the following approximate formula:

$$\frac{(1-2\beta^2 b^2)^n}{(1+2\beta^2 b^2)^{n+L+3/2}} = (-1)^n\frac{1}{(2\beta^2 b^2)^{L+3/2}}\frac{(1-1/2\beta^2 b^2)^n}{(1+1/2\beta^2 b^2)^{n+L+3/2}} \approx (-1)^n\frac{1}{(2\beta^2 b^2)^{L+3/2}}\exp\left\{-\frac{R_n^2}{4\beta^2 b^2}\right\}. \quad (43)$$

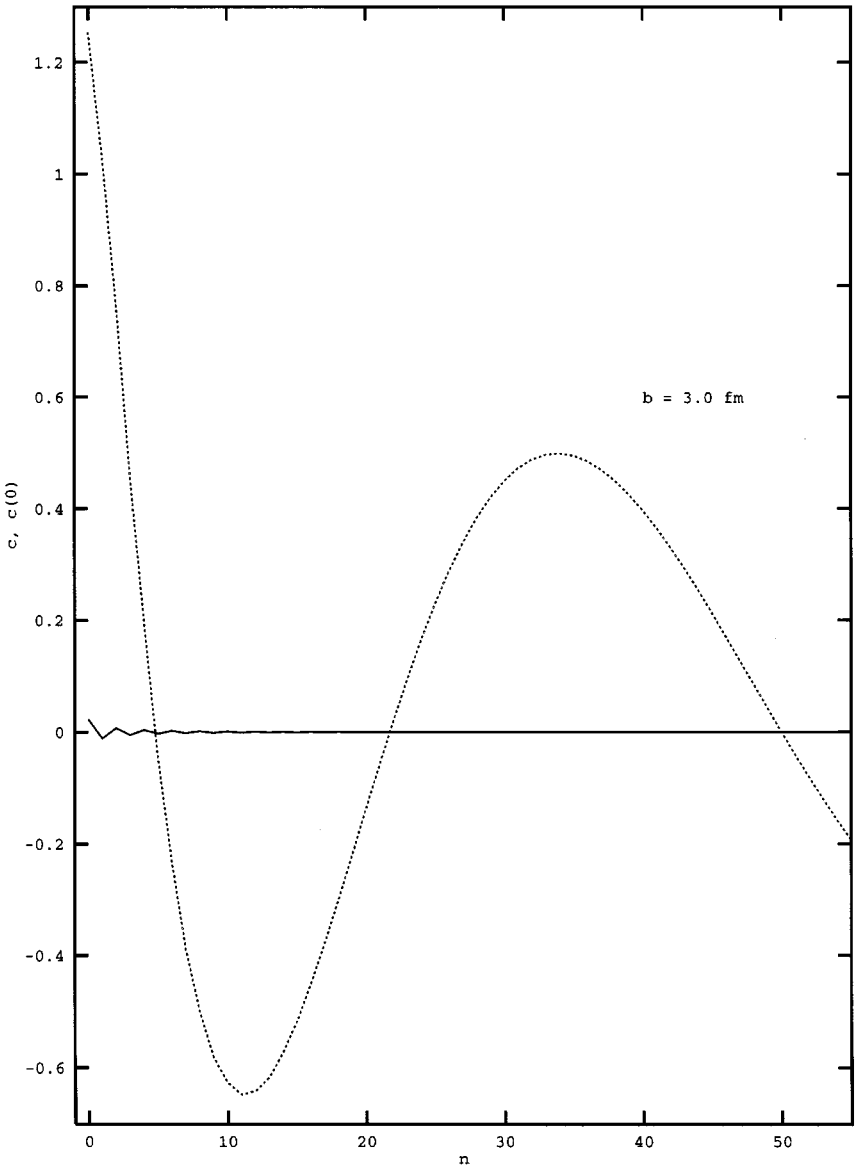

FIG. 10. c_n (dotted line) and $c_n^{(0)}$ (solid line) coefficients obtained in a calculation involving 100 basis states, with $b=3.0$ and an energy of 1 MeV.

The expansion coefficients can then be approximated by the second term in (38), which for very large values of b leads to the following asymptotic form of (37)

$$\langle n|\Psi\rangle \approx (-1)^n \sqrt{2} R_n^{L+1/2} b^L \int_0^\infty d\beta\, g(\beta) \frac{\exp\{-R_n^2/4\beta^2 b^2\}}{(2\beta^2 b^2)^{3/2}}. \tag{44}$$

Using an integral transformation, formula 11.4.29 of [12], the asymptotic form of the c_n for large b becomes

$$c_n = \langle n|\Psi\rangle \approx (-1)^n \frac{2}{\sqrt{\pi}} \sqrt{R_n} \int_0^\infty dr\, r^2 j_L\left(\frac{R_n}{b} r\right) \Psi(r), \tag{45}$$

$$= (-1)^n \frac{2}{\sqrt{\pi}} \sqrt{R_n} \Phi\left(\frac{R_n}{b}\right), \tag{46}$$

where Φ is the wave function in momentum representation.

For large values of the oscillator length b, the expansion coefficients of the wave function $\Psi(r)$ on an oscillator basis are thus proportional to the wave function in momentum space taken at discrete arguments which are the momentum values R_n/b. As oscillator functions in coordinate and momentum space only differ by a phase $(-1)^n$ and the argument ρ (which in coordinate space equals r/b and in momentum space equals kb), both wave functions $\Psi(r)$ in coordinate representation and $\Phi(p)$ in momentum representation have essentially the same expansion coefficients.

By integrating (45) by parts, assuming that $\Psi(r)$ is smooth and without singular points, and taking the leading asymptotic term for c_n (i.e., for $R_n \gg 1$), one obtains

$$\langle n|\Psi\rangle \approx (-1)^n \frac{1}{R_n^{3/2}} \Psi(0). \tag{47}$$

The same result can be obtained by considering that the wave functions $\Phi(p)$ of discrete and continuous spectrum states in momemtum space decrease at least as $1/p^2$. Substitution of this limiting factor in (46) again leads to (47)

Summing up one notes that the asymptotics of c_n are related to the wave function behavior in coordinate space: for small values of b the asymptotics are proportional to the

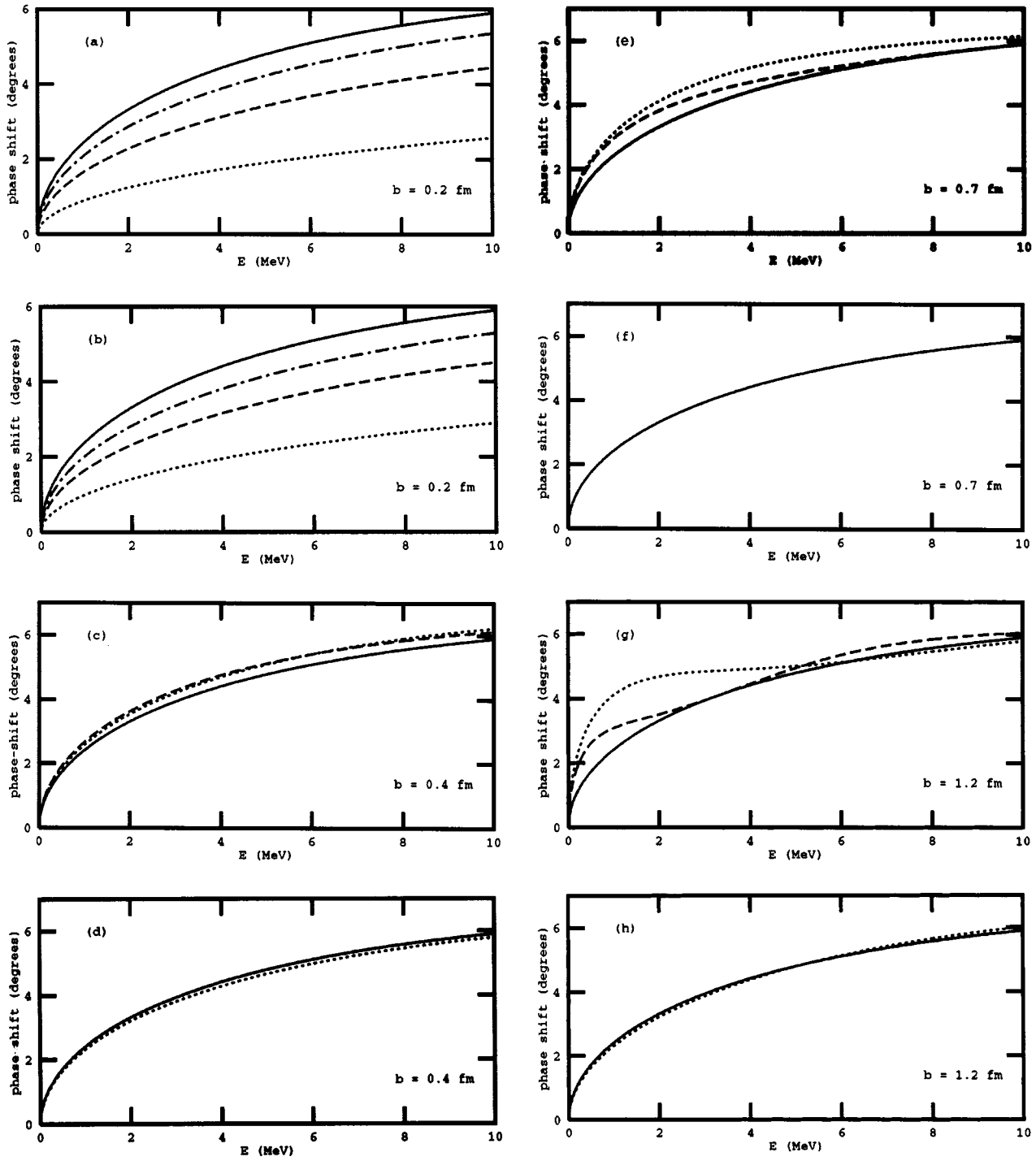

FIG. 11. Phase shift δ (degrees) as a function of energy, obtained with 5 (dotted line), 10 (dashed line), and 15 (dashed-dotted line) basis states. The solid line corresponds to the exact phase shift. Left side figures: phase shifts calculated with the original version of the dynamical equations. Right side figures: phase shifts calculated with the reformulated version of the dynamical equations.

wave function for large r, and for large values of b the asymptotics are proportional to the wave function in the vicinity of the origin.

2. Asymptotics of $\langle n|\hat{V}|\Psi\rangle$

Asymptotic expressions for the matrix elements $\langle n|\hat{V}|\Psi\rangle$ can be obtained in an analogous way as for $c_n=\langle n|\Psi\rangle$ by using the GC representation of the solution (33). We omit the details of the calculation, and only present the final results.

Small b values: for small b values (or better, small γ values), the matrix elements factorize as follows:

$$\langle n|\hat{V}|\Psi\rangle \approx \hat{V}(bR_n)\langle n|\Psi\rangle \approx \hat{V}(bR_n)\sqrt{2}\sqrt{R_n}\Psi(bR_n). \quad (48)$$

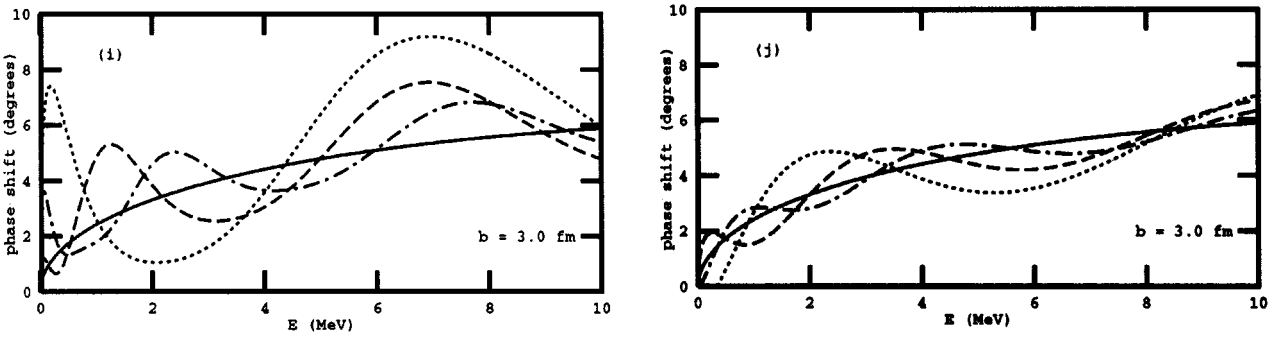

FIG. 11 (*Continued*).

One notices that the behavior of the matrix elements coincides with the one of the $\Psi(r)$, up to a trivial factor which is potential dependent. These results obtained for a general form of a short-range potential, are confirmed by the asymptotic form for $V_n^{(+)}$, evaluated earlier (29) for a Gaussian potential.

Large b values: for large values of b (or γ), the asymptotic form of the matrix elements $\langle n|\hat{V}|\Psi\rangle$ reduces to the integral

$$\langle n|\hat{V}|\Psi\rangle \approx (-1)^n \frac{2}{\sqrt{\pi}}\sqrt{R_n}\int_0^\infty dr\, r^2 j_L\left(\frac{R_n}{b}r\right)\hat{V}(r)\Psi(r) \tag{49}$$

or, in other words, to the convolution of the wave function with the potential in momentum representation

$$\langle n|\hat{V}|\Psi\rangle \approx (-1)^n \frac{2}{\sqrt{\pi}}\sqrt{R_n}\int_0^\infty d\tilde{k}\,\tilde{k}^2\hat{v}(k_n-\tilde{k})\Phi(\tilde{k}), \tag{50}$$

where $\hat{v}(k)$ and $\Phi_L(k)$ are the Fourier transforms of the potential $\hat{V}(r)$ and the wave function $\Psi(r)$, respectively.

These results for a general potential can again be checked by considering the corresponding form for $V_n^{(+)}$ obtained earlier with a Gaussian potential. Indeed, by calculating the integral

$$V_0\int_0^\infty dr\, r^2 j_L\left(\frac{R_n}{b}r\right)\exp\{-\gamma r^2\}j_L(kr), \tag{51}$$

where the unknown solution $\Psi(r)$ is substituted by $\Psi^{(+)}(k,r)=\sqrt{2/\pi}j_L(kr)$ (the ''free particle'' solution), one obtains (30), which is valid for both large b and n.

The matrix elements $\langle n|\hat{V}|\Psi\rangle$ can be evaluated in the asymptotic region by making the same assumptions concerning the behavior of $\Psi(r)$ as in the preceding section to obtain the asymptotic form of $c_n=\langle n|\Psi\rangle$. Expanding $\Psi(r)$ in a power series of r, keeping the first term $\Psi(0)r^L$ and integrating term by term in (49) leads to the following asymptotic form:

$$\langle n|\hat{V}|\Psi\rangle \approx (-1)^n \frac{2}{\sqrt{\pi}}\sqrt{R_n}\hat{v}\left(\frac{R_n}{b}\right)\Psi(0), \tag{52}$$

where the Fourier transform $\hat{v}(R_n/b)$ of the potential determines how fast the matrix elements decrease in terms of n.

B. New strategies for solving the AM equations

Based on the results obtained above, we can now suggest strategies for solving the dynamical equations of the AM, in those cases where the oscillator length b, or more exactly the ratio $\gamma=(b/a)^2$, is relatively large or small compared to the optimal value.

Small b values: we start from the Schrödinger equation in (1)

$$\sum_m \langle n|\hat{T}-E|m\rangle c_m+\langle n|\hat{V}|\Psi\rangle=0, \tag{53}$$

$$\sum_\mu \langle \nu|\hat{T}-E|\mu\rangle c_\mu+\langle \nu|\hat{V}|\Psi\rangle=0, \tag{54}$$

where the index n is connected with the internal region and ν with the asymptotic region, and N delimits the internal region. In the asymptotic region, we can use the asymptotic form (48) for the matrix elements

$$\langle \nu|\hat{V}|\Psi\rangle=\hat{V}(bR_\nu)c_\nu, \tag{55}$$

which yields

$$\sum_m \langle n|\hat{T}-E|m\rangle c_m+\langle n|\hat{V}|\Psi\rangle=0, \tag{56}$$

$$\sum_\mu \langle \nu|\hat{T}+\hat{V}(bR_\nu)-E|\mu\rangle c_\mu=0. \tag{57}$$

In the original version of the AM the asymptotic coefficients c_ν were given by (6), and obtained from a simple three term recurrence relation, due to the very selective coupling induced by the kinetic-energy operator between oscillator states. Instead of the original form, and based on (57), we propose a modified three term recurrence form, including the asymptotic behavior of the potential matrix elements in the diagonal term

$$\sum_\mu \langle \nu|\hat{T}+\hat{V}(bR_\nu)-E|\mu\rangle c_\mu=0 \tag{58}$$

or

$$[\langle \nu|\hat{T}|\nu\rangle+\hat{V}(bR_\nu)-E]c_\nu+\langle \nu|\hat{T}|\nu-1\rangle c_{\nu-1}+\langle \nu|\hat{T}|\nu+1\rangle c_{\nu+1}=0. \quad (59)$$

In the asymptotic region $c_\nu=c_\nu^{(+)}+\tan\delta c_\nu^{(-)}$, hence the system (59) should be solved independently for regular ($c_\nu^{(+)}$) and irregular ($c_\nu^{(-)}$) coefficients, with ''boundary'' conditions at starting remote points $\nu=N_a,N_a+1$

$$c_{\nu_0}^{(+)}=\sqrt{2R_\nu}j_L(kR_\nu), \quad (60)$$

$$c_{\nu_0}^{(-)}=\sqrt{2R_\nu}n_L(kR_\nu). \quad (61)$$

These modified asymptotic coefficients $c_\nu^{(+)}$ and $c_\nu^{(-)}$ should be considered when calculating the correspondingly modified $V_n^{(+)}$ and $V_n^{(-)}$ in the dynamical equations (21). The modified equations should then be solved for the phase shift δ and the coefficients of the internal region $c_n^{(0)}$.

Large b values: for large values of b, we consider the dynamical equations in the form (17), containing the $V_n^{(+)}$ and $V_n^{(-)}$ terms

$$\sum_{m=0}\langle n|\hat{H}-E|m\rangle c_m^{(0)}+V_n^{(-)}\tan(\delta)=-V_n^{(+)} \quad (62)$$

for the internal region ($n\leqslant N$), and

$$\sum_\mu \langle \nu|\hat{T}-E|\mu\rangle c_\mu+\langle \nu|\hat{V}|\Psi\rangle=0 \quad (63)$$

for $\nu>N$.

Substituting $c_\mu^{(0)}+c_\mu^{(+)}+\tan(\delta)c_\mu^{(-)}$ for c_μ in (63), and assuming that $c_\mu^{(+)}$ and $c_\mu^{(-)}$ satisfy the three-term recurrence relation (16), one obtains

$$\sum_\mu \langle \nu|\hat{T}-E|\mu\rangle c_\mu^{(0)}+\langle \nu|\hat{V}|\Psi\rangle=0. \quad (64)$$

Taking the asymptotic form (52) into account, one obtains the following equation for $c_\mu^{(a)}$:

$$\sum_\mu \langle \nu|\hat{T}-E|\mu\rangle c_\mu^{(a)}+(-1)^n\sqrt{R_n}v\left(\frac{R_n}{b}\right)=0, \quad (65)$$

where $c_\nu^{(0)}$ was substituted by

$$c_\nu^{(0)}=c_\nu^{(r)}+Wc_\nu^{(a)} \quad (66)$$

introducing the ''asymptotic'' coefficients $c_\nu^{(a)}$ and the ''residual'' coefficients $c_\nu^{(r)}$. All constants in the asymptotic form (52) were omitted and replaced by the global factor W to be determined. Equation (65) should now be solved subject to the boundary condition

$$c_\nu^{(a)}=0 \quad (67)$$

for $\nu=N_a,N_a+1$. Having obtained $c_\nu^{(a)}$, the equations for the internal region should be modified to take the substitution (66) into account

$$\sum_{m=0}\langle n|\hat{H}-E|m\rangle c_m^{(r)}+[V_n^{(a)}-Ec_n^{(a)}]W+V_n^{(-)}\tan(\delta)=-V_n^{(+)} \quad (68)$$

where $V_n^{(a)}$ now stands for the sum

$$V_n^{(a)}=\sum_{m=0}\langle n|\hat{H}|m\rangle c_m^{(a)}. \quad (69)$$

The meaning of the asymptotic coefficients $c_n^{(a)}$ can be most easily understood by considering the major part of the asymptotic behavior already in an intermediate n region. Indeed, for large b values, there is a very slow convergence of the results. This implies that the internal region extends towards very large n, with corresponding $c_n^{(0)}$ solutions probably very close (i.e., to first order) to the $c_n^{(a)}$.

Numerical application: To demonstrate how the (''small b'' and ''large b'') strategies accelerate the convergence, we again consider a Gaussian potential in the two limiting cases where (i) the oscillator radius is a factor of 5 less than the potential range, and (ii) the oscillator radius is a factor of 5 larger than the radius of the potential. Figure 12 compares the phase shifts, obtained at an energy of 1 MeV, obtained in the original, reformulated and asymptotic approaches.

In Fig. 13 we display the exact phase shifts and those obtained with our strategies using 5, respectively, 10, basis states. One notices that for the ''small b'' case, 5 basis functions yield almost exact results (within a precision less than 0.01%); by even considering only one basis function, the phase shift is obtained within a precision of 1%! In the original form the latter precision could only be reached by using more than 50 basis functions. For the ''large b strategy'' ($b/a=5$), the convergence speed is remarkably increased, although less spectacular than in the ''small b'' case. The number of states needed for an identical result in the original formulation (21) is about five times higher. The two strategies suggested are thus seen to significantly improve the convergence of the results and to reduce the computational efforts to obtain a desired precision.

By modifying the form of the asymptotic AM equations through inclusion of dynamical features as proposed and realized above for both small and large values of b, one is naturally led to the introduction of an ''intermediate region.'' This region distinguishes itself (i) from the ''internal region'' where the solutions are governed by the potential, and (ii) from the ''asymptotic region'' where the kinetic energy dominates the equations. In the intermediate region, the solutions are easily (i.e., in a numerically simple way) obtained. There are then actually two variational parameters to consider, N marking the border between the internal and intermediate region, and N_a marking the transition from the intermediate to the true asymptotic region. The larger or smaller is γ, the larger is the size (i.e., the difference N_a-N) of the intermediate region. The strategies proposed above for small and large values of γ have shown that, by considering a sufficiently large intermediate region (e.g.,

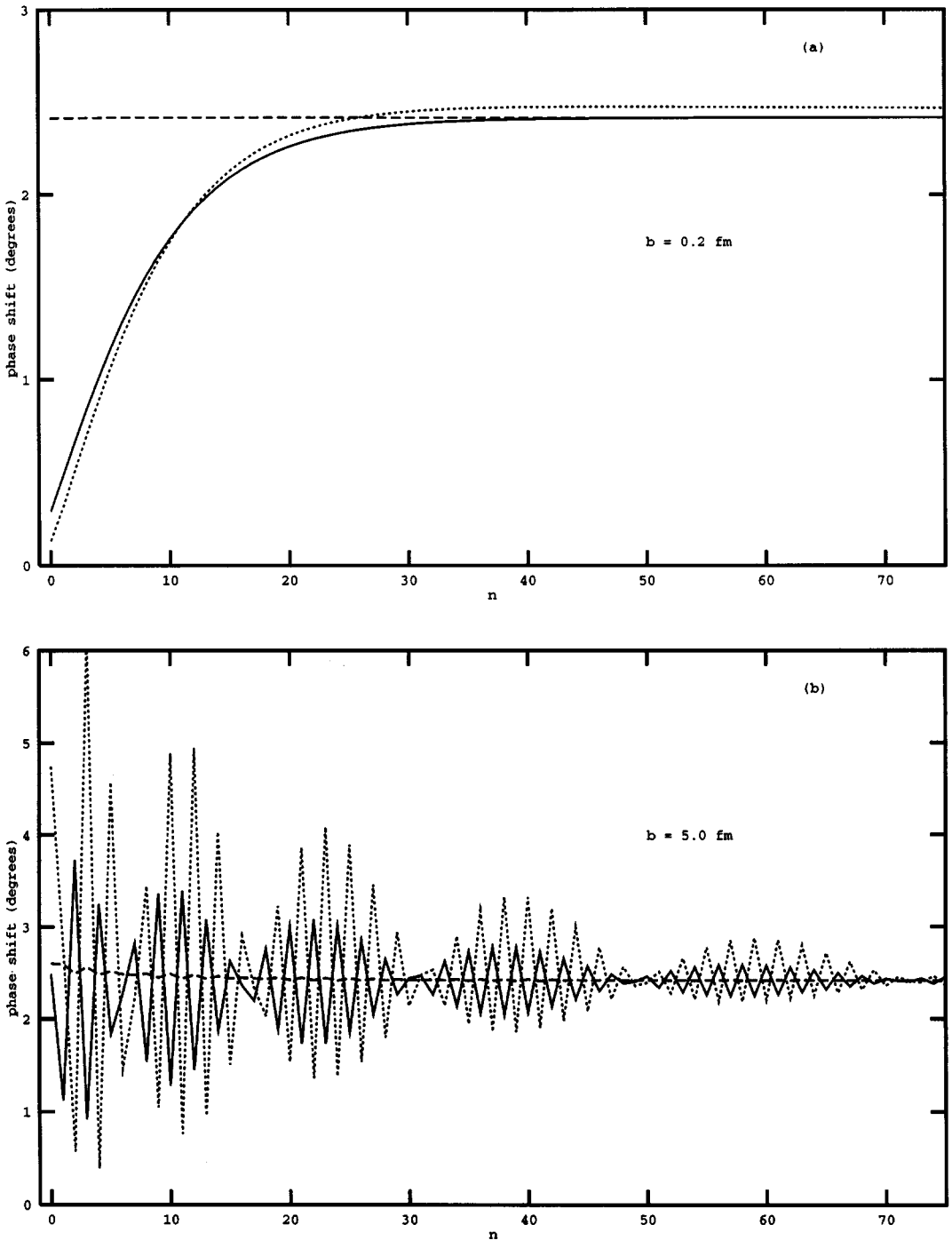

FIG. 12. Phase shifts at an energy of 1 MeV as a function of the number of basis states involved in the calculation. Dotted lines represent solutions of the original (''simple'') formulation, solid lines represent solutions of the reformulated version, and dashed lines represent solutions of the ''new strategies.''

$N_a = 500$), significantly reduces the range of the internal region, and dramatically decreases the computational effort to obtain converged results.

The intermediate region is characterized by a noticeable but nondominant presence of dynamical (i.e., potential) effects. These effects can be well approximated by asymptotic forms of both the expansion coefficients c_n and potential matrix elements $\langle n|\hat{V}|\Psi\rangle$. For small γ (long-range correlations), this leads to a redefinition of the equations of $c_n^{(+)}$ and $c_n^{(-)}$ by incorporation a potential term in the three term recurrence relation governing the true asymptotic behavior. For large γ (short-range correlations) one approximates part of the $c_n^{(0)}$ solution by its asymptotic behavior $c_n^{(a)}$. The latter are solutions of an inhomogeneous set of linear equations containing the Fourier transform of the potential, and as such accumulate the potential effects in the intermediate region. In the region of γ near to the optimal value, where fast converging solutions are obtained, there is no need for an inter-

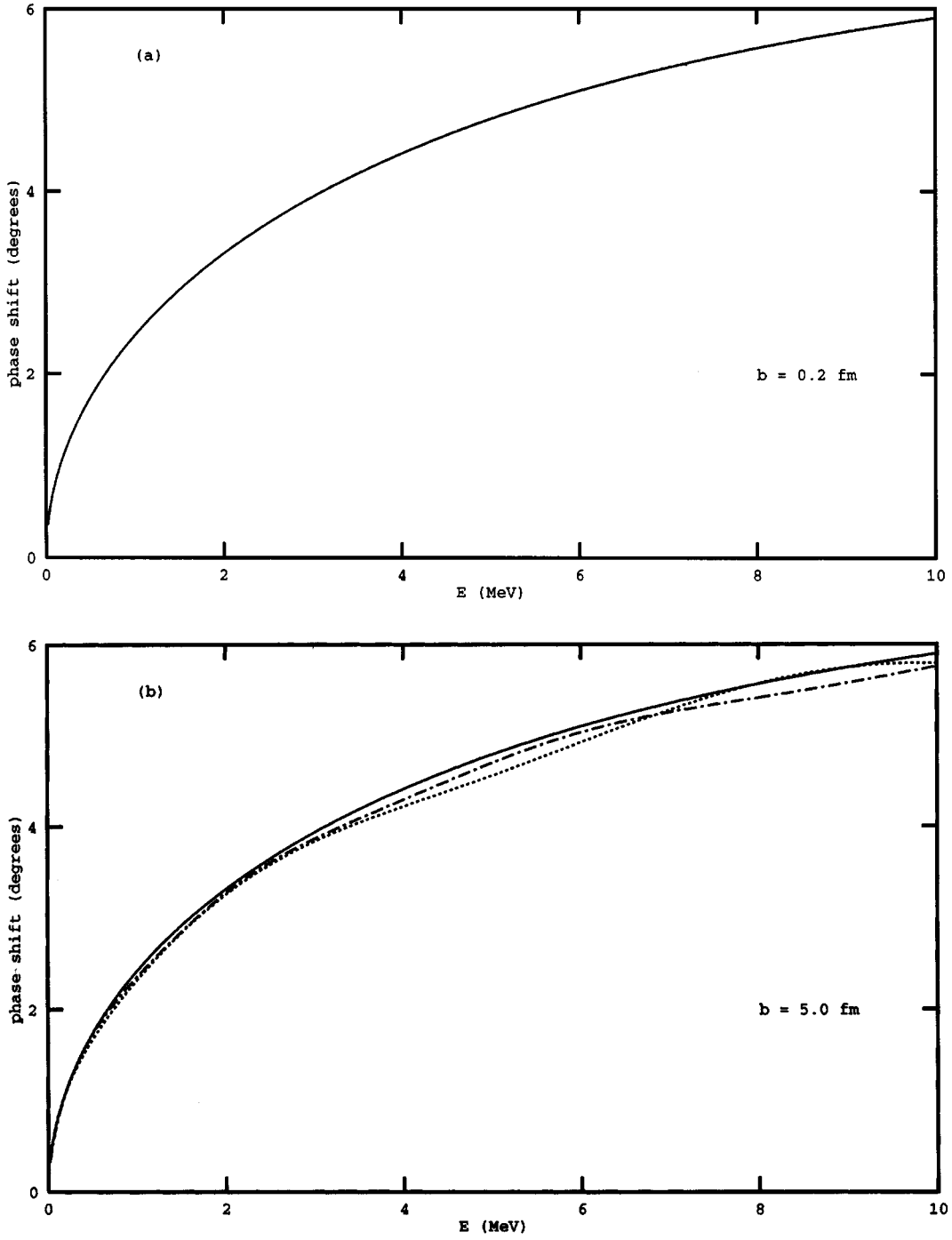

FIG. 13. Phase shifts in the energy range from 0 to 10 MeV for a ratio $b/a=0.2$, obtained in the ''small b strategy'' (top), and $b/a=5$, obtained in the ''large b strategy'' (bottom). Full lines show the exact solution, dotted (respectively, dashed) solutions are obtained with 5 (respectively, 10) basis states.

mediate region, and thus for an approximation of the dynamical equations; the values of N and N_a coincide in this case.

VI. CONCLUSIONS

By introducing the ''dynamical coefficients'' $V_n^{(+)}$ and $V_n^{(-)}$ we were able to suggest a form of the dynamical equations of the algebraic version of the resonating group method (AM). The dynamical coefficients allow one to determine oscillator basis parameters (oscillator length and number of basis functions) for obtaining otimally converging and stable solutions of these equations. It was shown that for an optimal parameter set 5 to 10 functions were sufficient to obtain results with a precision of more than 99.9%.

Our form of equations have also been shown to be a proper starting point for obtaining different solution strategies in parameter regions where slow convergence would occur. Indeed, in parameter regions were the oscillator length is much larger, respectively much smaller, than the optimal

one asymptotic approximations could be formulated by analyzing the AM equations. The latter can be easily implemented numerically, and have shown to dramatically improve the convergence of the solutions.

It was shown also that, if the oscillator radius is much smaller than the width of the potential, the expansion coefficients c_n of the wave function on the oscillator basis coincide with the wave function in coordinate space up to a simple factor. In the other limiting case, when the oscillator radius is much larger than the width of the potential, the expansion coefficients c_n were found to be proportional to the wave function in momentum space.

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APPENDIX

In this appendix the explicit form, and governing recurrence relations, of the dynamical coefficients $V_n^{(+)}$ and $V_n^{(-)}$ are calculated for a Gaussian potential. The following integrals should be evaluated:

$$V_n^{(+)}=V_0\int_0^\infty dr\, r^2\Phi_n(r)\exp(-r^2/a^2)\Psi^{(+)}(kr), \quad \text{(A1)}$$

$$V_n^{(-)}=V_0\int_0^\infty dr\, r^2\Phi_n(r)\exp(-r^2/a^2)\Psi^{(-)}(kr), \quad \text{(A2)}$$

where

$$\Psi^{(+)}=\sqrt{\frac{2}{\pi}}j_L(kr) \quad \text{and} \quad \Psi^{(-)}$$

is a solution of the inhomogeneous differential equation

$$(\hat{T}-E)\Psi^{(-)}=\beta_0\Phi_0(r), \quad \text{(A3)}$$

[β_0 is defined in eq. (13)], which can be represented in the integral form

$$\begin{aligned}\Psi^{(-)}&=\beta_0\int d\tilde{r}\,\tilde{r}^2G(r,\tilde{r})\Phi_0(\tilde{r})\\&=\beta_0\frac{2}{\pi}\int d\tilde{k}\int d\tilde{r}\,\tilde{r}^{\,2}\frac{j_L(\tilde{k}r)j_L(\tilde{k}\tilde{r})}{k^2-\tilde{k}^2}\Phi_0(\tilde{r})\\&=\beta_0\left(\frac{2}{\pi}\right)^{1/2}\int d\tilde{k}\,\frac{j_L(\tilde{k}r)c_0^{(+)}(\tilde{k})}{k^2-\tilde{k}^2}.\end{aligned} \quad \text{(A4)}$$

Integral (A1) is easily obtained by using formula 7.421.4 from [13] yielding

$$\begin{aligned}V_n^{(+)}&=(-1)^nV_0\frac{(1-2\gamma)^n}{(1+2\gamma)^{n+L+3/2}}q^L\\&\quad\times\exp\left(-\frac{1}{2}k^2\frac{1}{1+2\gamma}\right)N_{nL}L_n^{L+1/2}\left(\frac{k^2}{1-4\gamma^2}\right)\\&=V_0\frac{(1-2\gamma)^{n+L/2}}{(1+2\gamma)^{n+(L+3)/2}}\exp\left(\frac{1}{2}k^2\frac{\gamma}{1+2\gamma}\right)\\&\quad\times c_n^{(+)}(k/\sqrt{1-4\gamma^2}).\end{aligned} \quad \text{(A5)}$$

If $\gamma=1/2$, then

$$V_n^{(+)}=V_0N_{nL}\frac{1}{4}\frac{1}{n!}\left(\frac{k}{2}\right)^{2n+L+1/2}\exp\left(-\frac{1}{4}k^2\right). \quad \text{(A6)}$$

The second integral (A2), reduced to the form

$$V_n^{(-)}=\beta_0\int d\tilde{k}\frac{V_n^{(+)}(\tilde{k})c_0^{(+)}(\tilde{k})}{k^2-\tilde{k}^2} \quad \text{(A7)}$$

can be expressed through the $c_n^{(-)}$ coefficients

$$\begin{aligned}V_n^{(-)}&=V_0\frac{\exp\left(\frac{1}{2}q^2\frac{\gamma}{2\gamma+1}\right)}{(1+2\gamma)^{n+(L+3)/2}(1+\gamma)^{n+L/2}}\\&\quad\times\sum_{m=0}^{n}\frac{\Gamma(n+L+3/2)}{m!\Gamma(n-m+L+3/2)}\frac{N_{nL}}{N_{n-m,L}}\\&\quad\times[\gamma(1+2\gamma)]^mc_{n-m}^{(-)}(q),\end{aligned} \quad \text{(A8)}$$

where

$$q=k\left(\frac{1+\gamma}{1+2\gamma}\right)^{1/2}. \quad \text{(A9)}$$

New variables k' and $\tilde{k}'$

$$k'=\sqrt{\frac{1+\gamma}{1+2\gamma}}k,\tilde{k}'=\sqrt{\frac{1+\gamma}{1+2\gamma}}\tilde{k}, \quad \text{(A10)}$$

and the following relation for Laguerre polynomials [see [14], Vol. 2, formula 10.12(40)]

$$L_n^\alpha(\lambda x)=\sum_{m=0}^{n}\frac{\Gamma(n+\alpha+1)}{m!\Gamma(n-m+\alpha+1)}\lambda^{n-m}(1-\lambda)^mL_{n-m}^\alpha(x) \quad \text{(A11)}$$

were introduced in (A4) to obtain this result.

To obtain the recurrence relations for $V_n^{(+)}$ and $V_n^{(-)}$, we start from the equations for the functions $\Psi^{(+)}$ and $\Psi^{(-)}$

$$(\hat{T}-E)\Psi^{(+)}=0, \quad \text{(A12)}$$

$$(\hat{T}-E)\Psi^{(-)}=\beta_0\Phi_0(r). \quad \text{(A13)}$$

Multiplying both sides of these equations by $\Phi_n(r)V(r)$ and integrating, one obtains

$$\langle n|\hat{V}\hat{T}|\Psi^{(+)}\rangle - EV_n^{(+)} = 0, \tag{A14}$$

$$\langle n|\hat{V}\hat{T}|\Psi^{(-)}\rangle - EV_n^{(-)} = \beta_0\langle n|\hat{V}|0\rangle. \tag{A15}$$

One notices the similarity of the left-hand side of both equations, leading to identical recurrence relations for both type of coefficients. The matrix element $\langle n|\hat{V}|0\rangle$ for the Gaussian potential is

$$\langle n|\hat{V}|0\rangle = (-1)^n V_0 (1-z)^n z^{L+3/2}\left[\frac{\Gamma(n+L+3/2)}{n!\Gamma(L+3/2)}\right]^{1/2}, \tag{A16}$$

where

$$z = (\gamma+1)^{-1}. \tag{A17}$$

Using the commutation relations of the operators $\hat{T}$ and $\hat{V}$, or the explicit form of $V_n^{(+)}$, one finally obtains

$$(1+2\gamma)^2 T_{n,n+1} V_{n+1}^{(+)} + [(1-4\gamma^2)T_{n,n} - E]V_n^{(+)} + (1-2\gamma)^2 T_{n,n-1} V_{n-1}^{(+)} = 0, \tag{A18}$$

$$(1+2\gamma)^2 T_{n,n+1} V_{n+1}^{(-)} + [(1-4\gamma^2)T_{n,n} - E]V_n^{(-)} + (1-2\gamma)^2 T_{n,n-1} V_{n-1}^{(-)} = \beta_0\langle n|V|0\rangle. \tag{A19}$$

If in (A19) the potential is switched off [$V_0 = 1$ and $z = 1$ (or $\gamma = 0$)], the recurrence relations for $V_n^{(+)}$ and $V_n^{(-)}$ revert to these of $c_n^{(+)}$ and $c_n^{(-)}$ as is to be expected.

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