



On the Convergence of Reflectionless Approximations
to Confining Potentials

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Abstract

The construction of reflectionless potentials supporting a prescribed spectrum of Schrödinger bound states is discussed and related to the inverse problem for confining potentials. A simple formula is derived for the Jost solution in a one-dimensional reflectionless potential with N bound states. This leads to compact expressions for the potential and the bound-state wavefunctions in terms of the bound-state energies. For symmetric potentials, N -fold product formulas are obtained for bound-state wavefunctions and their slopes at the origin. Corresponding quantities in a confining potential are given by infinite products. Comparison of the finite-product and infinite-product expressions allows a demonstration of the convergence of the reflectionless results to the confining potential results as $N \rightarrow \infty$. Several sum rules satisfied by the reflectionless potential at the origin are applied to numerical studies of convergence.

I. INTRODUCTION

In a series of recent publications [1-3], several of us proposed a systematic procedure for using bound-state information to generate a sequence of approximations to a confining potential. The same procedure also yields approximations to the Schrödinger wavefunctions. In [1] the convergence of approximations to symmetric confining potentials in one dimension was studied numerically, with encouraging results. The closely-related problem of approximating a central potential for s-wave bound states in three dimensions was investigated in [2]. There an algorithm was presented for constructing from experimental data approximations to the (phenomenological) confining potential which binds massive quarks and antiquarks in meson systems such as J/ψ ($3 \text{ GeV}/c^2$) and T ($10 \text{ GeV}/c^2$). These approximations are determined by the masses and leptonic decay widths of the observed (spin-triplet) s-wave levels, in addition to two free parameters: the mass of the bound quarks and a fictitious continuum energy E_0 . The comparison of approximate potentials derived separately from information on the ψ and T families provided evidence that the interquark potential is flavor-independent [3]. We report in the present article new rigorous results and improvements in the numerical analysis.

The procedure developed in [1] involves the approximation of a symmetric, confining, one-dimensional potential $V(x) = V(-x)$ by a unique function $V_N(x; \mu, E_0)$ which satisfies the following three requirements:

(i) V_N supports precisely N bound states of a system with reduced mass μ . The bound-state energies coincide with the energies E_1, E_2, \dots, E_N of the N lowest-lying bound states in the potential $V(x)$.

$$(ii) \lim_{|x| \rightarrow \infty} V_N(x) = E_0(N).$$

(iii) For a system with reduced mass μ , the quantum-mechanical scattering determined by V_N is reflectionless.

We shall show that in the limit as N becomes infinite the Schrödinger wavefunctions and their first derivatives implied by the reflectionless approximation converge to the correct values at $x = 0$, so long as the ratio $E_o(N)/E_N$ approaches unity. In the course of this demonstration we shall also derive several sum rules that make possible a rather extensive numerical analysis of the large N behavior of $V_N(x = 0)$.

To arrive at these results we shall use general analytic properties of reflectionless systems in one dimension to establish simple closed formulae for the approximate wavefunctions and their derivatives at the origin in terms of the (even- and odd-parity) bound-state energies. These expressions will then be compared with infinite-product representations for the exact wavefunctions and their derivatives, obtained directly from analytic properties of the Schrödinger problem for the full confining potential.

An analogous approximation procedure was presented in [2] for the problem which is of direct physical interest to us: the reconstruction of a confining three-dimensional central potential $V(r)$. In this situation we approximate $V(r)$ by a unique function $V_{2n}(r; \mu, E_o)$ which meets these requirements:

(i) V_{2n} supports precisely n s-wave bound states of a system with reduced mass μ . Their energies and the squares of their normalized wavefunctions at the origin coincide with those of the n lowest-lying s-wave bound states in the potential $V(r)$.

(ii) $\lim_{r \rightarrow \infty} V_{2n}(r) = E_o(2n)$.

(iii) Regarded as a symmetric potential $V_{2n}(x) = V_{2n}(-x)$ in one dimension, the approximate potential defines a quantum-mechanical scattering problem with no reflection. The s-wave bound states of the central potential are identified with the odd-parity bound states of the one-dimensional problem. The normalized

wavefunctions at the origin ($r = 0$) of the three-dimensional s-wave states correspond to the slopes at $x = 0$ of the odd-parity wavefunctions of the one-dimensional problem.

When considered as a one-dimensional potential, V_{2n} also supports even-parity bound states which are fictitious from the standpoint of the three-dimensional central potential but nevertheless carry computational significance. The fictitious bound-state energies may be expressed as nontrivial algebraic functions of the s-wave bound-state energies and normalized wavefunctions at the origin. As a consequence, it is convenient to cast the three-dimensional problem in terms of the corresponding one-dimensional problem.

Before concluding this brief introduction, we wish to place the present work in the context of the general literature dealing with the inverse problem of the Schrödinger equation. Apparently little attention has been paid to approximation schemes of the kind we discuss. However, it has been shown by Grosse and Martin [4] that the full (infinite) set of s-wave energies and wavefunctions at the origin does uniquely determine a confining central potential which is integrable at $r = 0$. They have also presented a systematic procedure for constructing the even-parity bound-state energies of the symmetric problem in one dimension from the s-wave energies and wavefunctions at the origin of the three-dimensional problem. The question of whether all the energies of both parities uniquely characterize a symmetric potential in one dimension has been considered by Gasymov and Levitan [5], by Barcilon [6], and by Zakhariev, et al. [7], among others. The infinite product representations we shall derive make more graceful the connection between the one-dimensional and three-dimensional problems by expressing the derivatives of the odd-parity wavefunctions at $x = 0$ in terms of the odd-parity and even-parity bound-state energies. These representations amount to very natural extensions of the developments in ref. [5].

This paper is organized as follows. In the next Section we explain the general theory of reflectionless potentials which was set out in [1], following the ideas of Gel'fand and Levitan [8] and of Kay and Moses [9]. In Section III we specialize to the symmetric case and derive new expressions for wavefunctions and their derivatives at $x = 0$ and new sum rules for the potential at the origin. In earlier work [1,2] the reconstructed potential and its eigenfunctions were expressed in terms of determinants which were rather cumbersome in applications of practical importance. We have since learned how to bypass these large determinants. In addition, our discussion of the symmetric potential problem, which formerly made use of properties of soliton solutions of the Korteweg-de Vries equation [10], has been streamlined. The analytic theory of symmetric confining potentials is developed in Section IV. There infinite-product representations of the exact wavefunctions and their first derivatives at the symmetry point $x = 0$ are obtained, and the convergence of the one-dimensional reflectionless approximations to these quantities is established. Section V is devoted to numerical studies of the convergence of the reconstructed potential at the origin, and to an examination of the influence of the parameter E_0 . Some applications of the reflectionless approximation to quarkonium physics are discussed in Section VI. Section VII contains a résumé of our results and some parting remarks on future developments.

II. THE GENERAL REFLECTIONLESS POTENTIAL

In this Section we discuss some properties of the one-dimensional Schrödinger equation

$$\left(-\frac{\partial^2}{\partial x^2} + V(x) - V(\infty)\right) \phi(x, \zeta) = \zeta^2 \phi(x, \zeta) \quad (2.1)$$

in a general reflectionless potential $V(x)$. As in [1], we define Jost solutions ϕ_1 and ϕ_2 which are analytic in the upper-half ζ -plane with asymptotic behavior

$$\phi_1(x, \zeta) \sim e^{i\zeta x} \quad \text{as } x \rightarrow +\infty, \quad (2.2)$$

$$\phi_2(x, \zeta) \sim e^{-i\zeta x} \quad \text{as } x \rightarrow -\infty. \quad (2.3)$$

From these independent solutions to (2.1) we construct a meromorphic function $\Phi(x, \zeta)$ as

$$\Phi(x, \zeta) = \begin{cases} a^{-1}(\zeta) \phi_2(x, \zeta) e^{i\zeta x}, & \text{Im } \zeta > 0 \\ \phi_1^*(x, \zeta^*) e^{i\zeta x}, & \text{Im } \zeta < 0 \end{cases} \quad (2.4a)$$

$$(2.4b)$$

where $a^{-1}(\zeta)$ is the conventional transmission coefficient. The discontinuity of Φ across the real ζ -axis is proportional to the reflection coefficient and so vanishes for the reflectionless case we consider here.

In [1] the analytic properties of Φ were used to derive a set of linear algebraic equations for the normalized wavefunctions $\psi_n(x)$, $n = 1, 2, \dots, N$ of the bound states supported by the reflectionless potential $V(x)$. This procedure led to

explicit formulas for the potential $V(x)$ and the wavefunctions $\psi_n(x)$ in terms of $N \times N$ determinants that depend upon the bound-state energies. Numerical evaluation of these determinants is unappealing when N becomes large. However, explicit evaluation of the determinants for small values of N reveals extensive cancellations among terms, out of which emerge simplified expressions for $V(x)$ and for $\psi_n(x)$ exhibiting a systematic combinatorial pattern. Here we shall derive a general expression for the analytic function $\Phi(x, \zeta)$ from which the simplified forms for $V(x)$ and $\psi_n(x)$ follow directly.

By definition, $\Phi(x, \zeta)$ is meromorphic with poles on the positive-imaginary axis at $\zeta = i\kappa_n$, $n = 1, 2, \dots, N$ corresponding to bound states at $E_n = V(\infty) - \kappa_n^2$. The residues of these poles are proportional to the normalized bound-state wavefunctions. Hence we may express $\Phi(x, \zeta)$ in terms of its singularities [1] as

$$\Phi(x, \zeta) = 1 + i \sum_{n=1}^N \frac{c_n e^{i\kappa_n x}}{\zeta - i\kappa_n} \psi_n(x) \quad , \quad (2.5)$$

where c_n is determined by the asymptotic behavior of the bound-state wavefunction,

$$\psi_n(x) \underset{x \rightarrow \infty}{\sim} c_n e^{-\kappa_n x} \equiv \lambda_n(x) \quad . \quad (2.6)$$

Evaluated in the lower half-plane, at $\zeta = -i\kappa_n$, the function $\Phi(x, \zeta)$ is proportional to the bound-state wavefunction [1],

$$\Phi(x, -i\kappa_m) = \psi_m(x) / \lambda_m(x) \quad . \quad (2.7)$$

Combining eqns. (2.5) and (2.7), we obtain a system of N linear equations for the N wavefunctions $\psi_n(x)$, which may be represented as

$$\sum_{n=1}^N A_{mn} \psi_n = \lambda_m \quad , \quad (2.8)$$

where the matrix A is defined by

$$A_{mn} = \delta_{mn} + \frac{\lambda_m \lambda_n}{\kappa_m + \kappa_n} \quad . \quad (2.9)$$

Inverting eq. (2.8) as $\psi = A^{-1} \lambda$, we may rewrite eq. (2.5) in the form

$$\Phi(x, \zeta) = 1 + \sum_{m,n=1}^N \left(\frac{i \lambda_m}{\zeta - i \kappa_m} \right) (A^{-1})_{mn} \lambda_n \quad . \quad (2.10)$$

To deduce an explicit formula for $\Phi(x, \zeta)$, it is convenient to write

$$\Phi(x, \zeta) \equiv \mathcal{N}(x, \zeta) / \det A(x) \quad , \quad (2.11)$$

in recognition of the equivalence of A^{-1} to the matrix of cofactors of A divided by $\det A$. It follows from the definition of A that the function \mathcal{N} is a multinomial in the λ_n in which for each value of n only λ_n^0 and λ_n^2 can appear. We may therefore write

$$\mathcal{N} = \sum_S f_S(\{\kappa\}, \zeta) \prod_{p \in S} \lambda_p^2 \quad , \quad (2.12)$$

where the sum ranges over all subsets S of $\{1, 2, \dots, N\}$, including the null set and the full set. It will be useful below to notice that the contribution of the null set to (2.12) must be

$$f_{\phi}(\{\kappa\}, \zeta) = 1 \quad . \quad (2.13)$$

Comparison of (2.12) with the expression for \mathcal{N} obtained from (2.10) and (2.11) indicates that

$$f_S(\{\kappa\}, \zeta) = g_S(\{\kappa\}) \prod_{p \in S} \left(\frac{\zeta + i\kappa_p}{\zeta - i\kappa_p} \right) , \quad (2.14)$$

where the function g_S is independent of ζ . This may be seen as follows. According to eqns. (2.10-12), f_S must be equal to $\prod_{p=1}^N (\zeta - i\kappa_p)^{-1}$ times a polynomial of order N in ζ (in order that $\Phi(x, \zeta) \rightarrow 1$ as $\zeta \rightarrow \infty$). But note that, by (2.10), the residue in the pole of \mathcal{N} at $\zeta = i\kappa_p$ contains a factor λ_p^2 . Therefore the pole $(\zeta - i\kappa_p)^{-1}$ can only occur in f_S if $p \in S$, so that f_S must in fact be given by $\prod_{p \in S} (\zeta - i\kappa_p)^{-1}$ times a polynomial in ζ of order equal to the number of elements in the set S . Next rewriting eq. (2.7) as

$$\Phi(x, -i\kappa_p) = \frac{1}{\lambda_p} \sum_{q=1}^N (A^{-1})_{pq} \lambda_q , \quad (2.15)$$

we note that $\mathcal{N}(x, -i\kappa_p)$ is free of any terms containing a factor of λ_p^2 . Thus f_S must vanish at $\zeta = i\kappa_p$ for any $p \in S$. These requirements uniquely fix the ζ -dependence of f_S to be that displayed in (2.14).

Now let us determine $g_S(\{\kappa\})$. We note from (2.10) and (2.15) that

$$\lim_{\zeta \rightarrow i\kappa_p} (\zeta - i\kappa_p) \mathcal{N}(x, \zeta_p) = i\lambda_p^2 \mathcal{N}(x, -i\kappa_p) . \quad (2.16)$$

Evaluating both sides of (2.16) with the aid of (2.12) and (2.14), we are led by an inductive argument to the result

$$g_S(\{\kappa\}) = g_\phi \left[\prod_{p \in S} (2\kappa_p)^{-1} \right] \left[\prod_{(n \neq m) \in S} \left| \frac{\kappa_n - \kappa_m}{\kappa_n + \kappa_m} \right| \right] . \quad (2.17)$$

But, as indicated by (2.13) and (2.14), $g_\phi = 1$, so that

$$\mathcal{N}(x, \zeta) = \sum_S \left[\prod_{p \in S} \frac{\lambda_p^2}{2\kappa_p} \left(\frac{\zeta + i\kappa_p}{\zeta - i\kappa_p} \right) \right] \prod_{(n \neq m) \in S} \left| \frac{\kappa_n - \kappa_m}{\kappa_n + \kappa_m} \right| \quad (2.18)$$

Because $\Phi(x, \zeta) \rightarrow 1$ as $\zeta \rightarrow \infty$, $\det A$ must be the limit as $\zeta \rightarrow \infty$ of (2.18). Moreover, this implies that (2.18) itself can be written as a determinant. In summary, we have

$$\Phi(x, \zeta) = \frac{\det A(x, \zeta)}{\det A(x, \infty)} = \frac{\sum_S \left[\prod_{p \in S} \frac{\lambda_p^2}{2\kappa_p} \left(\frac{\zeta + i\kappa_p}{\zeta - i\kappa_p} \right) \right] \prod_{(n \neq m) \in S} \left| \frac{\kappa_n - \kappa_m}{\kappa_n + \kappa_m} \right|}{\sum_S \left[\prod_{p \in S} \frac{\lambda_p^2}{2\kappa_p} \right] \prod_{(n \neq m) \in S} \left| \frac{\kappa_n - \kappa_m}{\kappa_n + \kappa_m} \right|} \quad (2.19)$$

where the matrix $A(x, \zeta)$ is defined by

$$[A(x, \zeta)]_{pq} = \delta_{pq} + \frac{\lambda_p \left(\frac{\zeta + i\kappa_p}{\zeta - i\kappa_p} \right)^{\frac{1}{2}} \lambda_q \left(\frac{\zeta + i\kappa_q}{\zeta - i\kappa_q} \right)^{\frac{1}{2}}}{\kappa_p + \kappa_q} \quad (2.20)$$

Expressions for the bound-state wavefunctions now follow from the pole residues of (2.19), as

$$\psi_p(x) = \frac{\lambda_p}{D(x)} \sum_{S \not\ni p} \left[\prod_{q \in S} \frac{\lambda_q^2}{2\kappa_q} \left(\frac{\kappa_p - \kappa_q}{\kappa_p + \kappa_q} \right) \right] \prod_{(n \neq m) \in S} \left| \frac{\kappa_n - \kappa_m}{\kappa_n + \kappa_m} \right| \quad (2.21)$$

where

$$D(x) = \det A(x, \infty) = \sum_S \left[\prod_{p \in S} \frac{\lambda_p^2}{2\kappa_p} \right] \prod_{(n \neq m) \in S} \left| \frac{\kappa_n - \kappa_m}{\kappa_n + \kappa_m} \right| \quad (2.22)$$

The potential $V(x)$ may be recovered from $\Phi(x, \zeta)$ by noticing that [1]

$$\lim_{\zeta \rightarrow \infty} \zeta \frac{\partial \Phi}{\partial x}(x, \zeta) = \frac{i}{2} [V(x) - V(\infty)] \quad , \quad (2.23)$$

and using the fact (deduced from the numerator of (2.19)) that

$$\det A(x, \zeta) \underset{\zeta \rightarrow \infty}{\sim} D(x) - \frac{i dD/dx}{\zeta} + \mathcal{O}(\zeta^{-2}) \quad , \quad (2.24)$$

from which we recover [1]

$$V(x) = V(\infty) - 2 \frac{d^2}{dx^2} \ln D(x) \quad . \quad (2.25)$$

III. SYMMETRIC REFLECTIONLESS POTENTIALS

The results obtained in Section II are valid for an arbitrary reflectionless potential in one space dimension. A reflectionless potential which supports N bound states can be reconstructed uniquely in terms of the N binding energies $\kappa_n^2 = V(\infty) - E_n$ and N additional parameters c_n , defined in eq. (2.6). For the problem of a central potential in three dimensions which is of physical interest to us, it is appropriate to consider the case of a symmetric potential in one dimension [2]. We are thus led to consider the further simplifications of results of §II that follow from the symmetry requirement

$$V(x) = V(-x) \quad . \quad (3.1)$$

By convention we shall arrange the binding energies in descending order, $\kappa_1 > \kappa_2 > \dots > \kappa_N$, so that $E_1 = V(\infty) - \kappa_1^2$ refers to the ground-state energy, etc. Thus, the bound-state wavefunctions will satisfy the parity conditions

$$\psi_p(-x) = (-1)^{p+1} \psi_p(x) \quad ; \quad (3.2a)$$

and

$$\psi'_p(-x) = (-1)^p \psi'_p(x) \quad . \quad (3.2b)$$

Let us begin by evaluating $\Phi(x=0, \zeta)$ for a symmetric reflectionless potential. Since the even-numbered (odd parity!) wavefunctions vanish at $x=0$, inspection of (2.5) indicates that $\Phi(0, \zeta)$ has poles only at $\zeta = i\kappa_p$ for odd values of p . Hence $\Phi(0, \zeta)$ is given by $\prod_{p \text{ odd}} (\zeta - i\kappa_p)^{-1}$ multiplied by a polynomial in ζ of degree equal to the number of even-parity bound states: degree = $N/2$ if N is even, or degree = $(N+1)/2$ if N is odd. Consider first the even- N case. According to (2.7), $\Phi(0, -i\kappa_p) = 0$ for even values of p . With the asymptotic condition $\Phi \rightarrow 1$ as $\zeta \rightarrow \infty$, this requirement fixes the result

$$\Phi(0, \zeta) = \prod_{p=1}^N (\zeta + i\tau_p \kappa_p)^{\tau_p} \quad (N \text{ even}) \quad , \quad (3.3)$$

where

$$\tau_p \equiv (-1)^p \quad . \quad (3.4)$$

The case of odd N is most elegantly treated as a limiting case of N even with $\kappa_N \rightarrow 0$. From the asymptotic condition (2.6) it may be seen that normalization of

the wavefunction $\psi_N(x)$ requires that $\psi_N(x) \rightarrow 0$ for all x as $\kappa_N \rightarrow 0$. Thus, by (2.5) $\Phi(x, \zeta)$ for N even with $\kappa_N = 0$ is identical to $\Phi(x, \zeta)$ for $N - 1$ bound states. At $x = 0$ we therefore have

$$\Phi(0, \zeta) = \zeta \prod_{p=1}^N (\zeta + i\tau_p \kappa_p)^{\tau_p} \quad (N \text{ odd}) \quad (3.5)$$

Using (3.3) and (3.5) we may evaluate $\psi_p(0)$ and c_p for odd values of p . According to (2.5) and (2.7),

$$[\psi_p(0)]^2 = -i \lim_{\zeta \rightarrow i\kappa_p} [(\zeta - i\kappa_p)\Phi(0, \zeta)] \Phi(0, -i\kappa_p) \quad (3.6a)$$

$$= \frac{1}{2} (\kappa_p)^{-\tau_p N} \prod_{q \neq p} \left| \frac{\kappa_p^2 - \kappa_q^2}{\kappa_p - \kappa_q} \right|^{\tau_q}, \quad p \text{ odd} \quad (3.6b)$$

Again using (2.5) and (2.7) we have that

$$c_p^2 = [\lambda_p(0)]^2 = -i \lim_{\zeta \rightarrow i\kappa_p} [(\zeta - i\kappa_p)\Phi(0, \zeta)] / \Phi(0, -i\kappa_p) \quad (3.7a)$$

$$= 2\kappa_p \prod_{q \neq p} \left| \frac{\kappa_p + \kappa_q}{\kappa_p - \kappa_q} \right|, \quad p \text{ odd} \quad (3.7b)$$

Both (3.6b) and (3.7b) are valid for even and odd values of N . The expression (3.7b) and a similar expression (3.13b) below are precisely the conditions for a symmetric potential which were obtained in [1] by appealing to the properties of a complex of N Korteweg-deVries solitons.

Analogous results for even values of p may be deduced by considering the first derivative of Φ at $x = 0$. It is convenient to construct the function

$$G(x, \zeta) = \frac{\partial \Phi}{\partial x}(x, \zeta) - i\zeta \Phi(x, \zeta) \quad (3.8a)$$

$$= -i\zeta + \sum_{q=1}^N \lambda_q(x) \psi_q(x) + i \sum_{q=1}^N \frac{\lambda_q(x) \psi'_q(x)}{\zeta - i\kappa_q} \quad , \quad (3.8b)$$

where the last expression follows from (2.5). From (2.7) and (3.8a) we learn that

$$G(0, -i\kappa_p) = \psi'_p(0)/c_p \quad , \quad (3.9)$$

which vanishes for odd values of p in a symmetric potential. Equation (3.8b) shows that $G(0, i\kappa_p)$ has simple poles for p even, and that asymptotically $G(0, \zeta) \rightarrow -i\zeta$ as $\zeta \rightarrow \infty$. Consequently we may write

$$G(0, \zeta) = -i \prod_{p=1}^N (\zeta - i\tau_p \kappa_p)^{-\tau_p} \quad , \quad N \text{ odd} \quad . \quad (3.10)$$

As before, we may obtain an expression valid for even values of N by letting $\kappa_N \rightarrow 0$ in (3.10), whereupon

$$G(0, \zeta) = -i\zeta \prod_{p=1}^N (\zeta - i\tau_p \kappa_p)^{-\tau_p} \quad , \quad N \text{ even} \quad . \quad (3.11)$$

Using (3.10) and (3.11) we may now evaluate $[\psi'_p(0)]^2$ and c_p^2 for even values of p . According to (3.8b) and (3.9),

$$[\psi'_p(0)]^2 = -i \lim_{\zeta \rightarrow i\kappa_p} [(\zeta - i\kappa_p)G(0, \zeta)] G(0, -i\kappa_p) \quad (3.12a)$$

$$= \frac{1}{2} (\kappa_p)^{\tau_p} \prod_{q \neq p}^N \left| \kappa_p^2 - \kappa_q^2 \right|^{\tau_q} \quad , \quad p \text{ even} \quad , \quad (3.12b)$$

and

$$c_p^2 = -i \lim_{\zeta \rightarrow i\kappa_p} [(\zeta - i\kappa_p)G(0, \zeta)] / G(0, -i\kappa_p) \quad (3.13a)$$

$$= 2\kappa_p \prod_{q \neq p} \left| \frac{\kappa_p + \kappa_q}{\kappa_p - \kappa_q} \right|, \quad p \text{ even} \quad (3.13b)$$

The common expression (3.7b), (3.13b) for c_p^2 can be shown by explicit substitution in (2.25) to lead to a symmetric potential. From the definition (2.22) of $D(x)$ we find that

$$D(x) = \sum_S \exp \left[-2x \sum_{p \in S} \kappa_p \right] \Pi(S, \bar{S}) \quad , \quad (3.14)$$

where \bar{S} denotes the complement of the set S and

$$\Pi(S, \bar{S}) \equiv \prod_{\substack{m \in S \\ n \in \bar{S}}} \left| \frac{\kappa_m + \kappa_n}{\kappa_m - \kappa_n} \right| \quad . \quad (3.15)$$

Since $\Pi(S, \bar{S})$ is symmetric under the interchange of S and \bar{S} , we are free to combine terms in (3.14) to obtain

$$D(x) = \exp \left[-x \sum_{p=1}^N \kappa_p \right] \tilde{D}(x) \quad , \quad (3.16)$$

where

$$\tilde{D}(x) = \sum_S \Pi(S, \bar{S}) \cosh \left[x \left(\sum_{m \in S} \kappa_m - \sum_{n \in \bar{S}} \kappa_n \right) \right] \quad (3.17)$$

is manifestly symmetric in x . Hence

$$V(x) = V(\infty) - 2 \frac{d^2}{dx^2} \ln D(x) \quad (2.25)$$

$$= V(\infty) - 2 \frac{d^2}{dx^2} \ln \tilde{D}(x) \quad (3.18)$$

is symmetric as well because the exponential factor in (3.16) does not contribute to the second derivative of D .

Because eq. (3.7b), (3.13b) determine the N parameters c_p in terms of the binding energies, the reconstruction of a symmetric, reflectionless potential is specified uniquely by the N binding energies. It is this reduction in the number of parameters that makes it possible to contemplate physical applications of the inverse bound-state problem.

By substituting into (2.21) the expression for c_p , one can also obtain expressions for the bound-state wavefunctions which are themselves manifestly symmetric in x for odd values of p and antisymmetric in x for even values of p . Together with (3.17) and (3.18) these constitute a considerable simplification of the determinantal formulas derived in [1], both for the demonstration of symmetry properties and for practical computation.

A simple formula for $V(0)$ is obtained from eq. (2.23) with the aid of (3.3), (3.5), (3.10), and (3.11). We may write (2.23) as

$$V(0) = V(\infty) - 2i \lim_{\zeta \rightarrow \infty} \zeta \left. \frac{\partial \Phi}{\partial x} (x, \zeta) \right|_{x=0} \quad (3.19a)$$

$$= V(\infty) - 2i \lim_{\zeta \rightarrow \infty} [\zeta G(0, \zeta) + i \zeta^2 \Phi(0, \zeta)] \quad (3.19b)$$

A straightforward computation using the explicit forms for $G(0, \zeta)$ and $\Phi(0, \zeta)$ yields the result

$$V(0) = V(\infty) + 2 \sum_{p=1}^N (-1)^p \kappa_p^2 \quad (3.20)$$

This expression will find several applications in §V and §VI.

We conclude the formal development of this section by deriving two sum rules that relate $V(0)$ to the squares of wavefunctions or of slopes of wavefunctions at the origin. The first sum rule is based on the observation that

$$\phi(0, \zeta)\phi(0, -\zeta) = 1 - 2 \sum_{p=1}^N \frac{\kappa_p}{\zeta^2 + \kappa_p^2} [\psi_p(0)]^2 \quad (3.21)$$

and the second follows from

$$(1/\zeta^2)G(0, \zeta)G(0, -\zeta) = 1 + 2 \sum_{p=1}^N \frac{[\psi'_p(0)]^2}{\kappa_p(\zeta^2 + \kappa_p^2)} \quad (N \text{ even}) \quad (3.22)$$

Both of these expressions are derived most gracefully by examining the asymptotic behavior and the singularities of each side of the equations, using (2.5), (2.7), and (3.8) to determine the pole residues for the left-hand sides. Although eq. (3.22) is valid only for even values of N , it can be used in the now familiar way to obtain from the limit $\kappa_N \rightarrow 0$ results which hold for any value of N .

To derive the sum rules, we evaluate the left-hand sides of (3.21) and (3.22) using eqns. (3.3) and (3.11), and compare the coefficients of $(1/\zeta^2)$ on left-hand and right-hand sides, in the limit as $\zeta \rightarrow \infty$. From eq. (3.21) we find

$$\sum_{p=1}^N \tau_p \kappa_p^2 = -2 \sum_{p=1}^N \kappa_p [\psi_p(0)]^2 \quad (3.23)$$

whereas eq. (3.22) yields

$$\sum_{p=1}^N \tau_p \kappa_p^2 = -2 \sum_{p=1}^N \frac{[\psi'_p(0)]^2}{\kappa_p} \quad (\text{N even}) \quad (3.24)$$

To generalize (3.24) to include odd values of N, we need only note from (3.12b) that

$$\lim_{\kappa_N \rightarrow 0} \frac{[\psi'_N(0)]^2}{\kappa_N} = \frac{1}{2} \prod_{p \neq N} (\kappa_p^2)^{-\tau_p} \quad (3.25)$$

Using eq. (3.20) to express the left-hand sides of (3.23) and (3.24) in terms of the potential, we obtain the sum rules

$$V(0) = V(\infty) - 4 \sum_{p=1}^N \kappa_p [\psi_p(0)]^2 \quad , \quad (3.26)$$

and

$$V(0) = V(\infty) - 4 \sum_{p=1}^N \frac{[\psi'_p(0)]^2}{\kappa_p} + (\tau_N - 1) \prod_{p=1}^N (\kappa_p^2)^{-\tau_p} \quad (3.27)$$

The sum rules (3.26) and (3.27) will be applied in Section V to the numerical study of the convergence of reflectionless approximations to confining potentials at $x = 0$. The result (3.27) with N even is of particular importance for the three-dimensional problem because it depends only upon information about the physical s-wave levels (i.e. the odd-parity levels in one dimension). Equation (3.26) is a special case of a sum rule earlier derived by Gardner, Greene, Kruskal, and Miura [10].

To close this otherwise formal Section, we wish to illustrate the use of eq. (3.18) for the reconstruction of confining potentials. We display in Figs. 1-3 the 8-level one-dimensional reflectionless approximations to the symmetric linear, harmonic oscillator, and infinite square well potentials. In each case we have set

the reduced mass to $\mu = \frac{1}{2}$ and chosen the continuum energy $E_0(N) = V_N(\infty) = \frac{1}{2}(E_N + E_{N+1})$. The fidelity of approximation suggested in the figures is both remarkable and encouraging.

IV. CONVERGENCE TO WAVEFUNCTIONS AT THE ORIGIN

The results derived in the preceding Sections, especially (3.6b) and (3.12b), enable us to demonstrate the convergence of the reflectionless approximation for wavefunctions and their slopes at the origin. To accomplish this, we adapt to our present needs the program introduced by Grosse and Martin [4]. We consider solutions of the Schrödinger equation

$$-u''(x) + V(x)u(x) = Eu(x) \quad (4.1)$$

in a symmetric, confining potential

$$V(x) = V(-x) \quad , \quad (4.2)$$

$$\lim_{x \rightarrow \infty} V(x) = \infty \quad . \quad (4.3)$$

Under rather weak assumptions it can be shown [4] that there exists a solution $u(x, E)$ which behaves asymptotically like the (approximate) WKB wavefunction, i.e.

$$u(x, E) \underset{x \rightarrow \infty}{\sim} (V(x) - E)^{-1/4} \exp \left[- \int_{x_0}^x dy \sqrt{V(y) - E} \right] \quad , \quad (4.4)$$

where x_0 is the classical turning point, at which $V(x_0) = E$. The logarithmic derivative of the wavefunction at the origin,

$$R(E) \equiv \frac{u'(x, E)}{u(x, E)} \Big|_{x=0}, \quad (4.5)$$

plays a central role in the proof of convergence. By studying the properties of this function, we shall obtain infinite-product representations for the squares of bound-state wavefunctions and their slopes at the origin. The resulting infinite products are identical to the corresponding reflectionless approximations (3.6b) and (3.12b), in the limit of an infinite number of bound states ($N \rightarrow \infty$), provided that the parameter $E_0(N)$ is chosen properly. Thus the proof that reflectionless approximations converge to the exact wavefunctions and slopes at the origin reduces to a demonstration that certain infinite products exist.

It can be shown [4] that the function $R(E)$ is meromorphic, with alternating poles and zeroes lying on the real axis. The poles of $R(E)$ occur at the energies of the odd-parity bound states: $E = E_2, E_4, E_6, \dots$, and the zeroes occur at the energies of the even-parity levels: $E = E_1, E_3, E_5, \dots$. The residues of the poles in $R(E)$, which we shall require later to make contact with the reflectionless approximation, may be evaluated by constructing the Wronskian of solutions with energies E and $E + \Delta E$, which gives

$$\frac{d}{dE} \left(\frac{1}{R(E)} \right) \Big|_{E=E_p} = \frac{- \int_{-\infty}^{\infty} dx u^2(x, E_p)}{2 |u'(0, E_0)|^2}, \quad p \text{ even} \quad (4.6)$$

Similarly, the residue of the poles in $1/R(E)$ are found to be

$$\frac{d}{dE} R(E) \Big|_{E=E_p} = \frac{\int_{-\infty}^{\infty} dx u^2(x, E_p)}{2 |u(0, E_p)|^2}, \quad p \text{ odd} \quad (4.7)$$

If the potential $V(x)$ is integrable at the origin, the asymptotic behavior of R along the negative real axis is given by the WKB approximation of eqn. (4.4), which becomes valid down to $x = 0$ [4]. This yields

$$R(E) \underset{E \rightarrow -\infty}{\sim} -\sqrt{-E} + \mathcal{O}(1/\sqrt{-E}) \quad (4.8)$$

By taking the Wronskian of $u(x, E)$ with its complex conjugate, one obtains an important property of $R(E)$,

$$\frac{\text{Im}R(E)}{\text{Im} E} = \frac{\int_{-\infty}^{\infty} dx |u(x, E)|^2}{2 |u(0, E)|^2} > 0 \quad , \quad (4.9)$$

which is to say that the imaginary part of $R(E)$ is positive in the upper half-plane and negative in the lower half-plane. A function with this property is known as a Herglotz [11] or Pick [12] function. For our purposes, the most important attribute of such a function is that it grows no faster than $|E|$ and decreases no faster than $|E|^{-1}$. As a consequence, two Pick functions which have the same discontinuity across the real axis can differ only by a linear function $a + bE$. We shall use this fact to argue that $R(E)$ is specified uniquely by the positions of its poles and zeroes together with the asymptotic condition (4.8). This is a variation on the more familiar procedure of constructing an analytic function from its pole positions, pole residues, and asymptotic behavior which led to eq. (2.5).

Consider a Pick function $f(E)$ which has the same poles and zeroes as $R(E)$, namely

$$\left. \begin{aligned} f(E_p) &= 0 \quad , \quad p \text{ odd} \quad , \\ 1/f(E_p) &= 0 \quad , \quad p \text{ even} \quad , \end{aligned} \right\} \quad (4.10)$$

and which has the same asymptotic behavior as $R(E)$ along the negative real axis,

$$f(E) \underset{E \rightarrow -\infty}{\sim} -\sqrt{-E} + \mathcal{O}(1/-E) \quad . \quad (4.11)$$

We wish to demonstrate that these conditions ensure that $f(E) = R(E)$. To show this, let us compare $\ln f(E)$ and $\ln R(E)$. If we choose the branches of the logarithms so that both $\ln f$ and $\ln R$ are real in some interval (E_{2n-1}, E_{2n}) , then their discontinuities across the real axis are equal and alternate between $i\pi$ and zero:

$$\text{disc} [\ln f(E)] = \text{disc} [\ln R(E)] = \begin{cases} i\pi & -\infty < E < E_1 \\ 0 & E_1 < E < E_2 \\ i\pi & E_2 < E < E_3 \\ \vdots & \end{cases} \quad . \quad (4.12)$$

Moreover the fact that f and R are both Pick functions implies that

$$\left. \begin{array}{l} 0 \leq \text{Im} [\ln f(E)] \leq \pi \\ 0 \leq \text{Im} [\ln R(E)] \leq \pi \end{array} \right\} , \quad \text{Im } E > 0 \quad , \quad (4.13)$$

and that

$$\left. \begin{array}{l} 0 \geq \text{Im} [\ln f(E)] \geq -\pi \\ 0 \geq \text{Im} [\ln R(E)] \geq -\pi \end{array} \right\} , \quad \text{Im } E < 0 \quad . \quad (4.14)$$

Thus $\ln f$ and $\ln R$ are themselves Pick functions so that

$$\ln [f(E)] - \ln [R(E)] = a + bE \quad . \quad (4.15)$$

What is more, since by virtue of (4.13) and (4.14) the imaginary parts of $\ln f$ and $\ln R$ are bounded by π for all E , we must have $b = 0$. Finally, $a = 0$ follows from the asymptotic conditions (4.8) and (4.11). This proves that $f(E) = R(E)$.

Having established that $R(E)$ is specified uniquely by (4.9)-(4.11) we now construct the function explicitly. We shall show that it is none other than

$$f(E) \equiv \lim_{L \rightarrow \infty} \left\{ -C_L \prod_{n=1}^L \left(\frac{E - E_{2n-1}}{E - E_{2n}} \right) \right\} \quad , \quad (4.16)$$

where the sequence of positive numbers C_L satisfies

$$\lim_{L \rightarrow \infty} \frac{C_L}{\sqrt{E_{2L}}} = 1 \quad . \quad (4.17)$$

Provided that the limit exists (which will be verified below), the function (4.16) obviously has the desired poles and zeroes prescribed by (4.10). To show that (4.16) has the Pick function property (4.9), we note that all the pole residues in (4.16) are real and negative, so that we may write

$$f(E) = \lim_{L \rightarrow \infty} \left\{ -C_L + \sum_{n=1}^L \frac{r_n}{E - E_{2n}} \right\} \quad , \quad (4.18)$$

with $r_n < 0$. The property (4.9) follows immediately. To show that (4.16) exists and has the desired asymptotic behavior (4.11), it is convenient to rewrite the product in (4.16) as

$$\prod_{n=1}^L \left(\frac{E - E_{2n-1}}{E - E_{2n}} \right) = \exp \left\{ \ln \left(\frac{E - E_1}{E - E_2} \right) + \frac{1}{2} \ln \left(\frac{E - E_2}{E - E_{2L}} \right) + \sigma_L(E) \right\} , \quad (4.19)$$

where

$$\sigma_L(E) \equiv \sum_{n=1}^L \left[\ln \left(\frac{E - E_{2n-1}}{E - E_{2n}} \right) - \frac{1}{2} \ln \left(\frac{E - E_{2n-2}}{E - E_{2n}} \right) \right] . \quad (4.20)$$

Under fairly general conditions, the sum (4.20) is convergent as $L \rightarrow \infty$. Here we demonstrate this convergence for potentials that support energy levels with eigenvalues that are power-behaved for large principal quantum numbers,

$$E_n \sim \text{constant} \times n^\gamma . \quad (4.21)$$

This is the case, for example [13], for any potential which is power-behaved at large distances

$$V(x) \sim \text{constant} \times |x|^\nu . \quad (4.22)$$

Using this result we find that the large- n terms in (4.20) decrease more rapidly than n^{-1} , so that the sum over σ_L converges for large values of L . All of the L dependence of the product is therefore contained in the second term of the exponent in (4.19). Therefore we have shown that

$$\prod_{n=1}^L \left(\frac{E - E_{2n-1}}{E - E_{2n}} \right) = \frac{1}{\sqrt{E_{2L}}} B_L(E) , \quad (4.23)$$

where (for fixed values of E) $B_L(E)$ is finite and independent of L as $L \rightarrow \infty$. A sensible limit as $L \rightarrow \infty$ of the right-hand side of (4.16) will exist, provided only that C_L is proportional to $\sqrt{E_{2L}}$ for $L \rightarrow \infty$.

Thus the function $f(E)$ exists. Before identifying it with $R(E)$ defined by (4.5), we have only to check its asymptotic behavior as $E \rightarrow -\infty$. This is conveniently done using the representation (4.19). Using the WKB estimate (4.22) to determine the large- n terms in $\sigma_\infty(E) \equiv \lim_{L \rightarrow \infty} \sigma_L(E)$, we readily conclude that

$$\lim_{E \rightarrow -\infty} \sigma_\infty(E) = 0 \quad . \quad (4.24)$$

The large- E behavior of $f(E)$ then arises solely from the second term of the exponent in (4.19). The denominator $E - E_{2L}$ has already been absorbed in the $L \rightarrow \infty$ limit of (4.23). All that remains is the numerator, which contributes a factor $\sqrt{-E}$, so that

$$\lim_{E \rightarrow -\infty} f(E) = -\sqrt{-E} \lim_{L \rightarrow \infty} \frac{C_L}{\sqrt{E_{2L}}} \quad , \quad (4.25)$$

which satisfies the requirement (4.11), provided that the condition (4.17) is met.

Consequently we conclude that

$$R(E) = \lim_{L \rightarrow \infty} \left\{ -C_L \prod_{n=1}^L \left(\frac{E - E_{2n-1}}{E - E_{2n}} \right) \right\} \quad , \quad (4.26)$$

subject to (4.17).

The expressions (4.6) and (4.7) for the pole residues of $R(E)$ and $1/R(E)$ may now be used to construct infinite-product representations for the squares of the wavefunction and its slope at the origin. For normalized bound-state wavefunctions defined by

$$\psi_p(x) \equiv u(x, E_p) \left[\int_{-\infty}^{\infty} dx [u(x, E_n)]^2 \right]^{-1/2} \quad , \quad (4.27)$$

we find from (4.6), (4.7) and (4.26) that^{F1}

$$[\psi_p(0)]^2 = \lim_{L \rightarrow \infty} \left\{ \frac{1}{2\sqrt{E_{2L}}} (E_{p+1} - E_p) \prod_{\substack{n=1 \\ 2n-1 \neq p}}^L \left(\frac{E_p - E_{2n}}{E_p - E_{2n-1}} \right) \right\}, \quad p \text{ odd} \quad (4.28)$$

and

$$[\psi'_p(0)]^2 = \lim_{L \rightarrow \infty} \left\{ \frac{\sqrt{E_{2L}}}{2} (E_p - E_{p-1}) \prod_{\substack{n=1 \\ 2n \neq p}}^L \left(\frac{E_p - E_{2n-1}}{E_p - E_{2n}} \right) \right\}, \quad p \text{ even} \quad (4.29)$$

Let us now rewrite the reflectionless approximations (3.6b) and (3.12b) in forms that are easily compared with these results. We have, for even values of N ,

$$[\psi_p(0)]^2|_N = \frac{1}{2\sqrt{E_o(N) - E_p}} \prod_{q \neq p}^N |E_p - E_q|^{\tau_q}, \quad p \text{ odd} \quad (4.30)$$

and

$$[\psi'_p(0)]^2|_N = \frac{\sqrt{E_o(N) - E_p}}{2} \prod_{q \neq p}^N |E_p - E_q|^{-\tau_q}, \quad p \text{ even} \quad (4.31)$$

with $\tau_q = (-1)^q$. Hence the $N \rightarrow \infty$ limit of the reflectionless approximation to $[\psi_p(0)]^2$ and $[\psi'_p(0)]^2$ gives precisely the same result as a confining potential with the same spectrum, provided that

$$\lim_{N \rightarrow \infty} \frac{E_o(N)}{E_N} = 1 \quad (4.32)$$

This is what we set out to prove.

V. NUMERICAL ILLUSTRATIONS OF CONVERGENCE

The discussion in Section IV has made apparent the importance of a proper choice of the lowest continuum energy $E_0(N)$ for an N -level approximation to a confining potential and its Schrödinger wavefunctions. The requirement (4.32) that $\lim_{N \rightarrow \infty} (E_0(N)/E_N) = 1$ guarantees that the approximate wavefunctions and their first derivatives converge to the exact results at $x = 0$.

The requirement that

$$\lim_{N \rightarrow \infty} V_N(0) = V(0) \quad (5.1)$$

imposes a much more stringent constraint upon $E_0(N)$. It is our purpose in this Section to explore the circumstances under which convergence to the exact value of the potential at the origin can be achieved. To do so, we shall examine calculations based upon three realizations of the reflectionless approximation technique:

- (i) reconstruction of a symmetric potential from its energy levels of both odd and even parity, characterized by the sum rule

$$V_N(0) = E_0(N) + \frac{1}{\mu} \sum_{p=1}^N (-1)^p \kappa_p^2 ; \quad (3.16)$$

- (ii) reconstruction of a symmetric potential from its even-parity energy levels and their wavefunctions at the origin, corresponding to the sum rule

$$V_N(0) = E_0(N) - \frac{2}{\mu} \sum_{p=1}^N \kappa_p |\psi_p(0)|^2 , \quad \text{for odd } N; \quad (3.22)$$

(iii) reconstruction of a symmetric potential from its odd-parity energy levels and the slopes of their wavefunctions at the origin, represented by the sum rule

$$V_N(0) = E_0(N) - \frac{2}{\mu} \sum_{p=1}^N \frac{|\psi'_p(0)|^2}{\kappa_p}, \quad \text{for even } N. \quad (3.23)$$

All of these methods are of course identical if one uses the values of κ_p , $|\psi_p(0)|^2$, and $|\psi'_p(0)|^2$ associated with an N-level symmetric reflectionless potential, rather than only the N lowest levels of a confining potential. However, in practice it may be necessary or desirable to approximate a confining potential on the basis of mixed information. For the quarkonium problem discussed in the Introduction it is the information contained in the third sum rule (3.27) which is accessible to experiment.

We shall consider three examples of confining potentials (linear, harmonic oscillator, and infinite square well), always assuming that $2\mu = 1$. For the linear potential,

$$V(x) = |x|, \quad (5.2)$$

the energy eigenvalues are given by the zeroes of Airy functions:

$$\left. \begin{aligned} \text{Ai}'(-E_n) &= 0 & (n = 1, 3, 5, \dots) & , \\ \text{Ai}(-E_n) &= 0 & (n = 2, 4, 6, \dots) & ; \end{aligned} \right\} \quad (5.3)$$

and the normalized wavefunctions at the origin are [13]

$$\left. \begin{aligned} |\psi_n(0)|^2 &= 1/(2E_n) & (n = 1, 3, 5, \dots) & , \\ |\psi'_n(0)|^2 &= 1/2 & (n = 2, 4, 6, \dots) & . \end{aligned} \right\} \quad (5.4)$$

The bound-state energies of the harmonic oscillator potential,

$$V(x) = x^2, \quad (5.5)$$

are the odd integers

$$E_n = 2n - 1 \quad (n = 1, 2, 3, \dots), \quad (5.6)$$

and the normalized wavefunctions at the origin are [14]

$$\left. \begin{aligned} |\psi_{2p+1}(0)|^2 &= \frac{1}{2^{2p}\sqrt{\pi}} \frac{(2p)!}{(p!)^2} & , \\ |\psi'_{2p+2}(0)|^2 &= \frac{1}{2^{2p-1}\sqrt{\pi}} \frac{(2p+1)!}{(p!)^2} & , \end{aligned} \right\} \quad (5.7)$$

where $p = 0, 1, 2, \dots$. The infinite square well

$$V(x) = \begin{cases} 0, & |x| < \pi/2 \\ \infty, & |x| > \pi/2 \end{cases} \quad (5.8)$$

supports bound states at

$$E_n = n^2 \quad (n = 1, 2, 3, \dots) \quad , \quad (5.9)$$

with wavefunctions

$$\left. \begin{aligned} |\psi_n(0)|^2 &= 2/\pi & (n = 1, 3, 5, \dots) & , \\ |\psi'_n(0)|^2 &= 2n^2/\pi & (n = 2, 4, 6, \dots) & . \end{aligned} \right\} \quad (5.10)$$

In reference [1] the lowest continuum energy was chosen as

$$E_o(N) = \frac{1}{2}(E_N + E_{N+1}) \quad , \quad (5.11)$$

which was adopted in calculating the one-dimensional reflectionless approximations shown in Figs. 1-3. With this choice, $V_N(0) = 0$ for all values of N for the harmonic oscillator potential, and visually excellent approximations result for all three examples. Let us now examine more quantitatively the convergence of the reflectionless approximation to $V(0)$.

For the three examples under consideration, $V(0) = 0$. The values of $V_N(0)$ which follow from the choice (5.11) for $E_o(N)$ are shown in Fig. 4(a) for reflectionless approximations to the linear potential (5.2) based upon the three sets of bound-state information characterized by sum rules (3.20), (3.26), and (3.27). The approximations based upon the energy levels of both parities (plotted at all the integers) and upon the even-parity energy levels and wavefunctions (plotted at the odd integers) tend with increasing N toward the true value $V(0) = 0$. In contrast, the approximation based upon the odd-parity energy levels and slopes of their wavefunctions drifts away from $V(0) = 0$. All three approximations yield values of

$V_N(0)$ which differ from the correct value by amounts that are diminishing fractions of the nominal depth of the potential as measured by $E_0(N)$. This is shown in Fig. 4(b).

An analogous situation may be observed for the harmonic oscillator potential (5.5) in Fig. 5. As already noted, the approximation to $V(0)$ based upon the bound-state energies of both parities is exact for this case. The even-parity approximation (3.26) again tends toward $V(0) = 0$, while the odd-parity approximation (3.27) departs from the true value somewhat more rapidly than was the case for the linear potential. The deviations of $V_N(0)$ from zero are once more decreasing fractions of $E_0(N)$.

Approximations to the infinite square well (5.8) manifest rather similar behavior, as illustrated in Fig. 6. This time the one-dimensional approximation (3.20) leads to

$$V_N(0) = (\frac{1}{2})(-1)^N, \quad (5.12)$$

and the even-parity approximation (3.26) departs gradually from $V(0) = 0$. Both of these provide excellent fractional approximations to the depth of the potential. The odd-parity approximation departs significantly from the true value of $V(0)$ but shows signs (confirmed by more extensive numerical studies) of converging in the fractional sense.

What is to be learned from these numerical exercises? At least in some circumstances, the reflectionless approximations to confining potentials are seen to converge to $V(0)$ as the number of included bound states tends to infinity. The rate of convergence depends upon the particular approximation employed and upon the precise choice of $E_0(N)$ within the allowed interval, as we shall soon demonstrate in

more detail. For the examples we have considered, the numerical studies have not indicated that the odd-parity approximation converges to $V(0)$ when $E_0(N)$ is chosen according to (5.11). The numerical experiments do not, of course, prove that convergence does not occur. The confining potentials we have considered as examples all have $V'' \geq 0$, which is to say $|\psi'_{p+1}(0)|^2 \geq |\psi'_p(0)|^2$. Consequently the largest term in the sum rule (3.27) is the final term, $|\psi'_N(0)|^2 / \overline{E_0(N) - E_N}$, which is exquisitely sensitive to the choice of $E_0(N)$. Approximations to concave-downward potentials, or to potentials for which $|\psi'_p(0)|^2$ is a decreasing function of p , are likely to prove less strongly affected by the choice of $E_0(N)$.

An alternative to (5.11) would be the choice of $E_0(N)$ to guarantee that $V_N(0) = V(0)$ for all N . (This condition is not physically motivated, for it relies upon information that is inaccessible to experiment!) According to the discussion in §IV, fine-tuning E_0 will not alter the fact of convergence to the Schrödinger wavefunctions (although it will influence the rate of convergence). It is straightforward to choose $E_0(N)$ to ensure that $V_N(0) = V(0)$ for the one-dimensional approximation. To see this, let us rewrite the sum rule (3.20) as

$$V_N(0) = E_0(N)(-1)^N + 2 \sum_{p=1}^N (-1)^{p+1} E_p, \quad (5.13)$$

which leads to

$$E_0(N) = V(0)(-1)^N + 2 \sum_{p=1}^N (-1)^{N-p} E_p. \quad (5.14)$$

It follows from (5.14) that

$$E_0(N) = 2N = \frac{1}{2}(E_N + E_{N+1}) \quad (5.15)$$

is the appropriate choice for the harmonic oscillator potential (as we knew) and that

$$E_o(N) = N(N+1) = (E_N E_{N+1})^{1/2} = \frac{1}{2}(E_N + E_{N+1}) - \frac{1}{2} \quad (5.16)$$

ensures that $V_N(0) = V(0)$ for the infinite square well. Similarly $E_o(N)$ may be expressed in terms of sums and differences of zeroes of Airy functions for the linear potential. The values of $E_o(N)$ for which $V_N(0) = V(0)$ at finite values of N are plotted in Figs. 7-9 for the linear, harmonic oscillator, and square well potentials. Note that $V_N(0) = V(0)$ is not a trivial condition when eq. (3.22) (even-parity approximation) or eq. (3.23) (odd-parity approximation) is used, because $E_o(N)$ appears nonlinearly. The even-parity approximation to the linear potential cannot reproduce $V_N(0) = V(0) = 0$ for any real choice of $E_o(N)$, for finite values of N . In all the other cases examined, a suitable choice of $E_o(N)$ can be made.

Many numerical studies of the rate of convergence of the reflectionless approximation to quantum mechanical observables suggest themselves, but we are not yet able to provide a comprehensive description of the convergence problem. We will, however, cite one amusing consequence of the choice (5.11) for $E_o(N)$. Application of the one-dimensional approximation to the ground state of the square well using (3.4) for the wavefunction at the origin leads to a rapidly-converging expression for π :

$$\pi = \lim_{n \rightarrow \infty} S_n \quad , \quad (5.17)$$

where

$$S_n \equiv \begin{cases} \frac{4}{\sqrt{n(n+1) - \frac{1}{2}}} \frac{(3^2 - 1)(5^2 - 1)\dots(n^2 - 1)}{(2^2 - 1)(4^2 - 1)\dots((n-1)^2 - 1)} & , \quad n: \text{ odd} \\ 4\sqrt{n(n+1) - \frac{1}{2}} \frac{(3^2 - 1)(5^2 - 1)\dots((n-1)^2 - 1)}{(2^2 - 1)(4^2 - 1)\dots(n^2 - 1)} & , \quad n: \text{ even} \end{cases} \quad (5.18)$$

The first three terms in the sequence of approximations are $S_1 = 1.040 \pi$, $S_2 = 0.995 \pi$, $S_3 = 1.001 \pi$, which exhibit a rapid convergence indeed!

As a final application of the sum rules (3.20), (3.26), and (3.27), let us investigate how well a potential singular at the origin is reproduced by the reflectionless approximation. Consider the Coulomb potential

$$V(r) = -1/r \quad (5.19)$$

in three dimensions, for which the limit of the continuum energy is naturally chosen as

$$E_o = \lim_{N \rightarrow \infty} E_o(N) = 0 \quad (5.20)$$

The S-wave bound-state energies of the Schrödinger equation are

$$E_n = -1/4n^2 \quad (n = 1, 2, 3, \dots) \quad (5.21)$$

and the odd-parity wavefunctions of the corresponding one-dimensional problem satisfy

$$|\psi'_{2n}(0)|^2 = 1/4n^3 \quad (5.22)$$

It is straightforward to sum the (infinite) series (3.27) in this case; one finds

$$V_\infty(0) = -2 \sum_{n=1}^{\infty} \frac{1}{n^2} = -\frac{\pi^2}{3} \approx -3.29 \quad (5.23)$$

Thus the odd-parity reflectionless approximation leads to a very deep, but finite, representation of the Coulomb potential. Of course, even for a non-singular potential, we would not expect to reproduce $V(0)$ exactly if V is not confining, since information from the continuous part of the spectrum has been ignored.

VI. PHYSICAL APPLICATIONS AT $x = 0$

In the preceding Sections of this article we have elaborated and applied the reflectionless approximation to confining potentials. The new formal results of this work, which concern the Schrödinger wavefunctions and the reconstructed potential at the origin, have made possible a systematic (if still incomplete) investigation of the convergence of the method. In this Section our intent is considerably different: we now apply the new formal results to the problem of reconstructing the interquark potential from the properties of quarkonium states.

The program we envisage [2, 3] for the quarkonium system entails the reconstruction of a spin-triplet, s-wave potential from the masses and leptonic-decay widths of the 3S_1 ($Q\bar{Q}$) levels. The leptonic width of an n^3S_1 quarkonium state of mass M_n is related by the van Royen-Weisskopf formula [15]

$$\Gamma(\mathcal{V}_n^0 \rightarrow e^+e^-) = \frac{16\pi N_c}{3} e_Q^2 \frac{\alpha^2 |\psi_n(0)|^2}{M_n^2} \quad (6.1)$$

to the wavefunction at the origin. Here N_c is the number of colors (3 for ordinary quarks), e_Q is the quark charge in units of the proton charge, and $\alpha \approx 1/137$ is the fine-structure constant. Experimental information about an infinite number of bound states will of course not be available.^{F2} What we hope to achieve is therefore not an exact reproduction of the interquark potential, but a faithful representation in the region of space probed by a small number of bound states. Numerical experiments reported in [1] and extended by Figs. 1-3 encourage this approach.

The odd-parity reflectionless approximation characterized by the sum rule (3.27) makes use of the available information. The masses of the quarkonium levels correspond to the energies E_2, E_4, \dots of the odd-parity levels in one dimension. The three-dimensional wavefunction Ψ_n is connected to the one-dimensional odd-parity wavefunction ψ_{2n} by

$$|\Psi_n(0)|^2 = (1/2\pi) |\psi_{2n}'(0)|^2 \quad . \quad (6.2)$$

The experimental information, supplemented by the continuum parameter E_0 and the mass m_Q of the bound quark, specifies the approximate potential. Since the quark mass is not known from other information, we arrive at a two-parameter family of potentials which reproduce the spectrum of s-wave bound states. By comparing with experiment the predictions these potentials entail for other observables (e.g. the masses of orbital excitations) we may select a favored potential from among the possibilities. This has been done [2] for the charmonium family, by using the $\psi(3095)$ and $\psi'(3686)$ masses and leptonic widths to generate a family of potentials which were winnowed on the basis of the center of gravity of the 2^3P_J levels and the properties of the epsilon resonances.

It is useful for computation to reexpress the wavefunction information in terms of (fictitious) even-parity energy levels of the related one-dimensional problem. This may be done by inverting the connection (3.12b) between the bound-state energies and the wavefunctions, which can be transcribed as

$$|\Psi_n(0)|^2 = \frac{(m_Q)^{3/2}}{4\pi} (E_0 - M_n)^{1/2} \frac{\prod_{k=1}^N |M_n - E_{2k-1}|}{\prod_{p \neq n} |M_n - M_p|}, \quad (6.3)$$

when the potential is reconstructed from N (three dimensional) physical levels. The set of N equations of the form (6.3) in the N unknowns $E_1, E_3 \dots E_{2N-1}$ is conveniently solved in practice by iteration, or by minimizing the function

$$\chi^2(\{E_{2k-1}\}) = \sum_{n=1}^N \left[|\Psi_n(0)|_{\text{input}}^2 - |\Psi_n(0)|_{\{E_{2k-1}\}}^2 \right]^2 \quad (6.4)$$

using standard numerical search techniques.

By substituting eq. (6.1) and (6.2) into the sum rule (3.23) we arrive at an expression for

$$V(0) = E_0 - \frac{3}{2N_c e_Q^2 \alpha^2 m_Q^{3/2}} \sum_{n=1}^N \left[M_n^2 \Gamma_n / \sqrt{E_0 - M_n} \right] \quad (6.5)$$

which makes explicit the dependence of $V(0)$ upon the properties of the bound quark, and upon E_0 . For a given set of vector meson masses and leptonic widths the potential is deeper, the smaller is the quark's color charge N_c or electric charge e_Q or mass m_Q . Radiative corrections to (6.1), which could well be appreciable, may alter these conclusions quantitatively but not qualitatively. As E_0 approaches the highest level M_N from above, the potential becomes infinitely deep.

VII. SUMMARY AND OUTLOOK

A totally satisfying theory of heavy quarkonium states would provide a description from first principles of the quark-antiquark binding. It is generally held that the interquark force directly reflects the properties of the nonabelian glue of quantum chromodynamics, but reliable calculations are lacking. The overall phenomenological success of nonrelativistic potential models for the ψ and T states [16,17] encourages the belief that future considerations will center upon the determination of a static, interquark potential. In [1] and [2], a systematic procedure whereby reflectionless approximations to the potential could be constructed directly from the masses and leptonic widths of s-wave bound states was described. An approximate potential thus reconstructed from information on the ψ family provided a number of predictions for the T states that were subsequently confirmed by experiment. Later [3] a potential determined from the properties of the T states alone yielded direct evidence, free from the bias of a specific assumed parametrization, for flavor-independence of the interaction. When more complete data are available for the T system, we expect these inverse methods to produce an extremely faithful reproduction of the true potential.

The adoption of reflectionless approximations is of course a matter of calculational simplicity, but it is also a very natural restriction for confining potentials in which the spectral data consist entirely of bound-state parameters. Indeed, we have seen in §IV that in a confining potential bound-state wavefunctions and their slopes at the origin can be written as infinite products which are limiting cases of finite-product representations for the same quantities in a reflectionless potential. The numerical experiments reported in [1] and in this article indicate, moreover, that the reflectionless approximation procedure converges rapidly for any reasonably well-behaved potential. Although it may be doubted that in the real

world of light quarks and finite flavor thresholds the issue of mathematical convergence is of any great significance, the numerical studies show that excellent local approximations are achieved with only a few bound states.

Quarkonium aside, the convergence of the reflectionless approximation to confining potentials is a topic of interest in mathematical physics. The discussion in §IV represents the beginning of an analytic treatment of convergence. Our accomplishments are nontrivial, but rather limited: pointwise convergence has been demonstrated only for wavefunctions and their slopes at the origin in a symmetric potential. It goes without saying that statements about the potential and wavefunctions away from the symmetry point are to be desired.

In our investigation of convergence, as in the earlier work of Grosse and Martin [4], a central rôle was played by the logarithmic derivative of the (asymptotically damped) Schrödinger wavefunction. From its analytic properties, this function was shown to have an infinite-product representation, which yielded infinite-product representations for the wavefunctions and their slopes at the origin. An analogous rôle was played in the case of reflectionless potentials by the logarithmic derivative $G(0, \zeta)/\Phi(0, \zeta)$ of the Jost solution $\Phi(x, \zeta)e^{-i\zeta x}$ at the origin. This similarity suggests that in view of the representation (2.19) for $\Phi(x, \zeta)$, the wavefunction in the confining potential could be expressed as the $N \rightarrow \infty$ limit of a ratio of N -dimensional determinants. If this could be shown, convergence results away from the origin would be forthcoming immediately. An investigation along these lines may lead to a more complete understanding of the relationship between the inverse spectral problems for reflectionless and confining potentials.

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FOOTNOTES

- F¹ Expressions (4.28) and (4.29) closely resemble ones derived in Ref. 7 under a different set of boundary conditions.
- F² The experimental difficulty is self-evident. Perhaps more importantly, the single-channel potential model description is untrustworthy above the (flavor) threshold for decay of $(Q\bar{Q})$ quarkonium states into $(Q\bar{q}) + (\bar{Q}q)$ meson pairs.

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CAPTIONS

- Fig. 1: The eight-level reflectionless approximation to the linear potential $V(x) = |x|$. Bound-state energies are indicated by the broken lines.
- Fig. 2: The eight-level reflectionless approximation to the harmonic oscillator potential $V(x) = x^2$. Bound-state energies are indicated by the broken lines.
- Fig. 3: The eight-level reflectionless approximation to the infinite square well potential $V(x) = \{0, |x| < \pi/2; \infty, |x| > \pi/2\}$. Bound-state energies are indicated by the broken lines.
- Fig. 4: (a) The value of the reflectionless approximation to the linear potential $V(x) = |x|$ at the origin, given by the sum rules (3.16), (3.22), and (3.23). For all three cases, the choice $E_0(N) = \frac{1}{2}(E_{N+1} + E_N)$ has been made. The approximation (3.16) based on the bound-state energies of both parities is plotted (top curve) at all (integer) values of the number N of bound states. At odd values of N the approximation (3.22), which makes use of the even-parity bound-state energies and the values of even-parity wavefunctions at the origin, is plotted (middle curve). The approximation (3.23), based on the energies of the odd-parity bound-states and the values of the slopes of the odd-parity wavefunctions at the origin, is plotted (bottom curve) at the even integers. (b) Fractional errors $V_N(0)/E_0(N)$ of the approximations.
- Fig. 5: Same as Fig. 4, for the harmonic oscillator potential $V(x) = x^2$.
- Fig. 6: Same as Fig. 4, for the infinite square well potential.

Fig. 7: The value of $E_0(N) - E_N$ which yields $V_N(0) = V(0) = 0$ for a finite value of N for the linear potential is displayed as a fraction of the level splitting $E_{N+1} - E_N$. The set of points at all integers corresponds to the approximation (3.16). The set plotted at the even integers refers to (3.23). In this case, no real choice of $E_0(N)$ yields $V_N(0) = 0$ for the even-parity approximation (3.22), which would be plotted on the odd integers.

Fig. 8: Same as Fig. 7, for the harmonic oscillator potential.

Fig. 9: Same as Fig. 7, for the infinite square well potential.

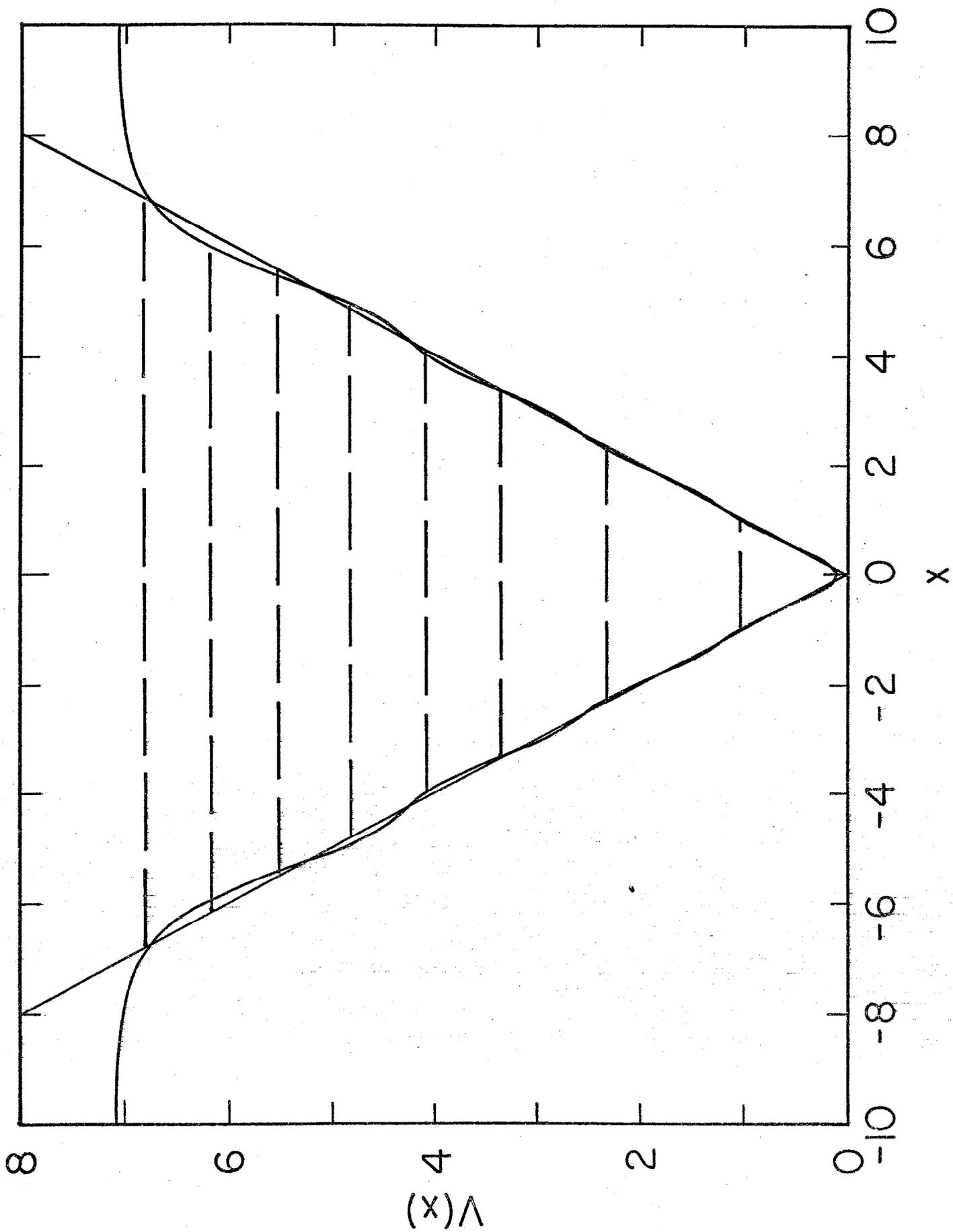
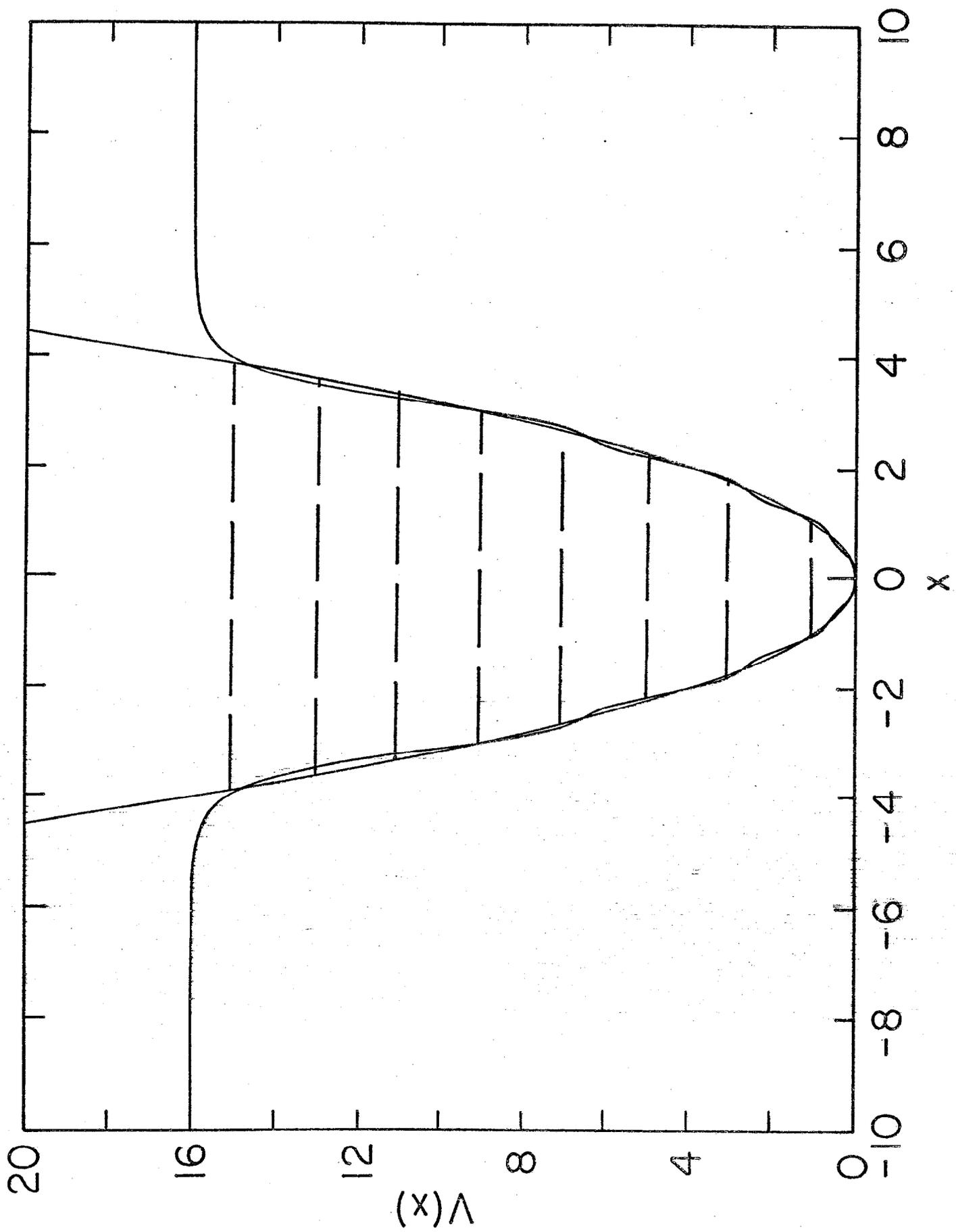
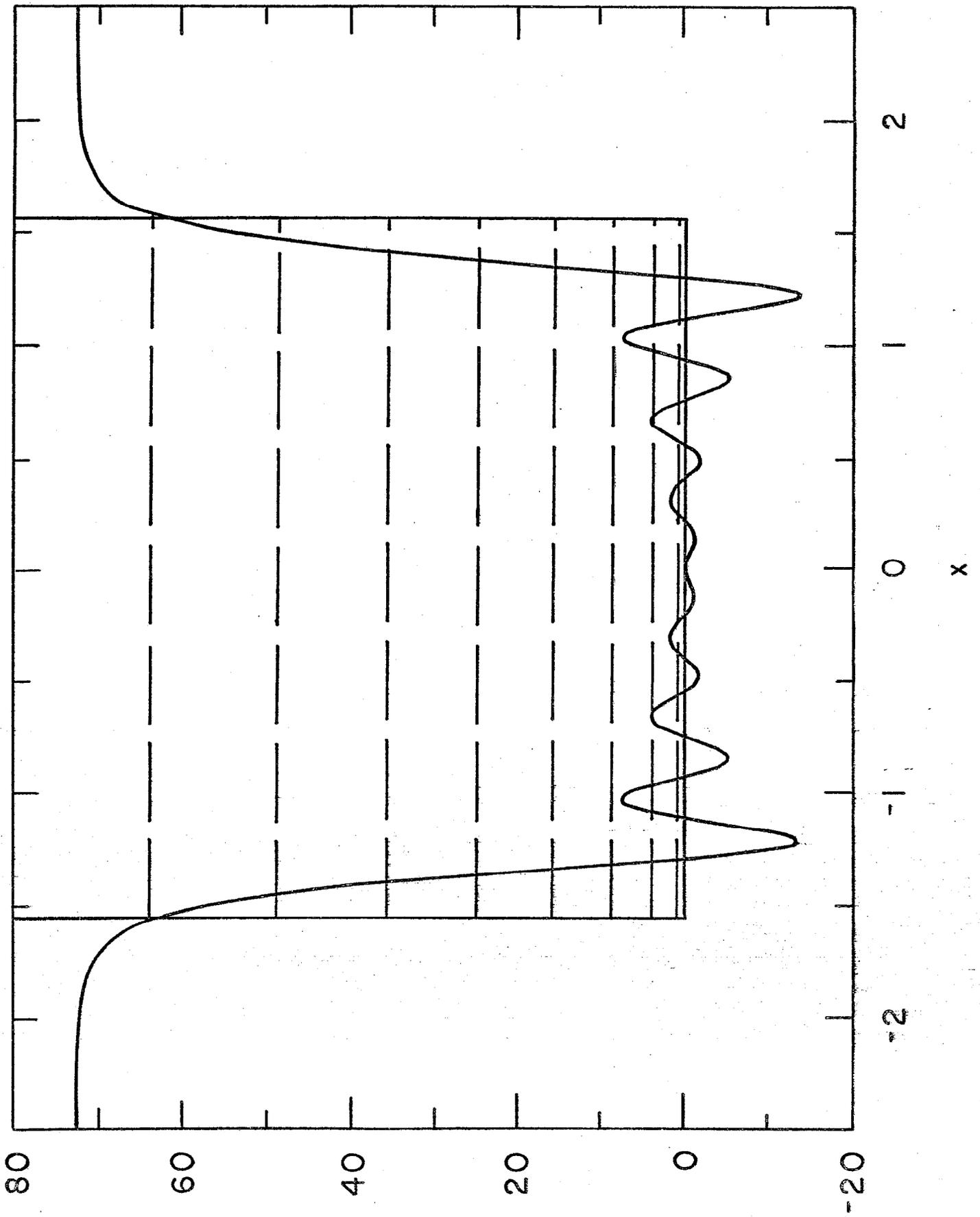


Fig. 1





$\Lambda(x)$
Fig. 2

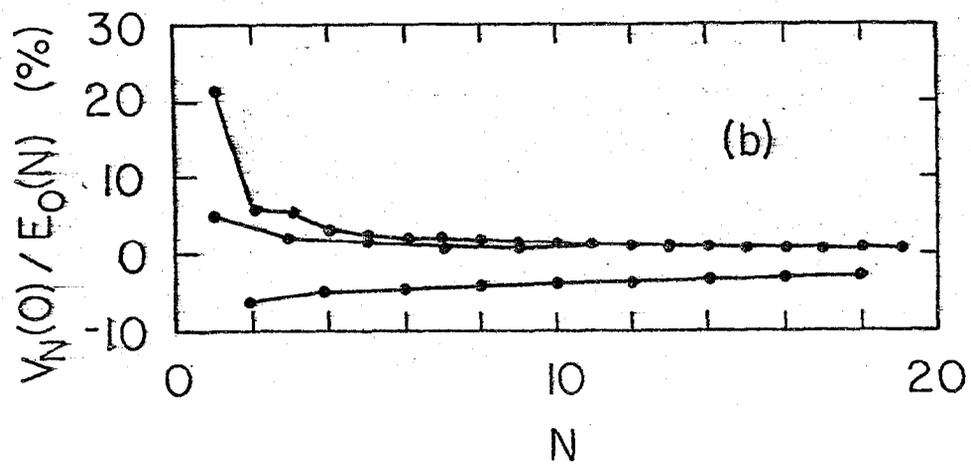
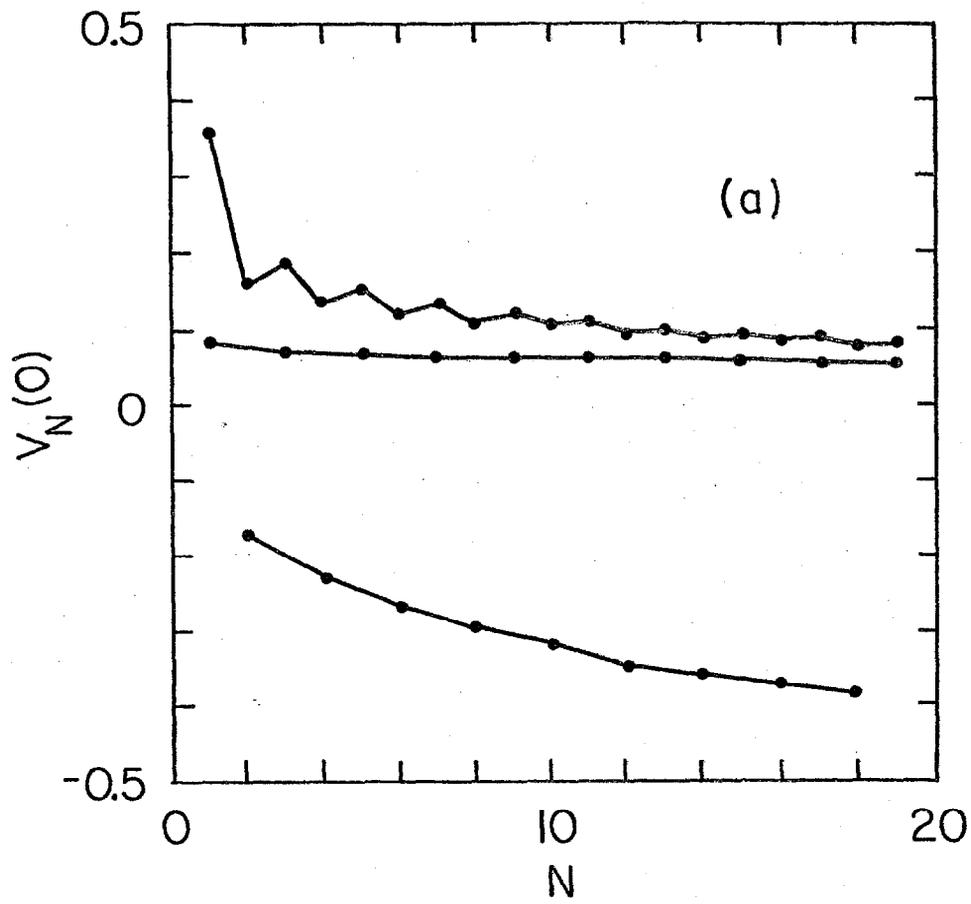


Fig. 4

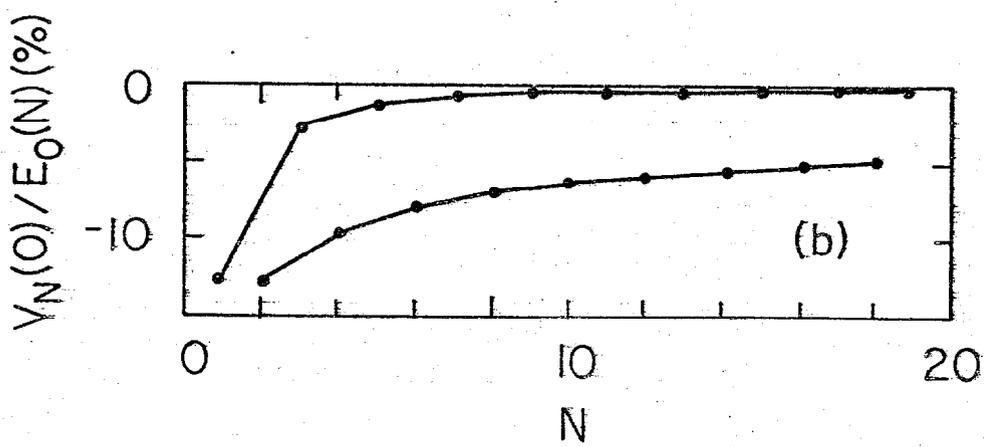
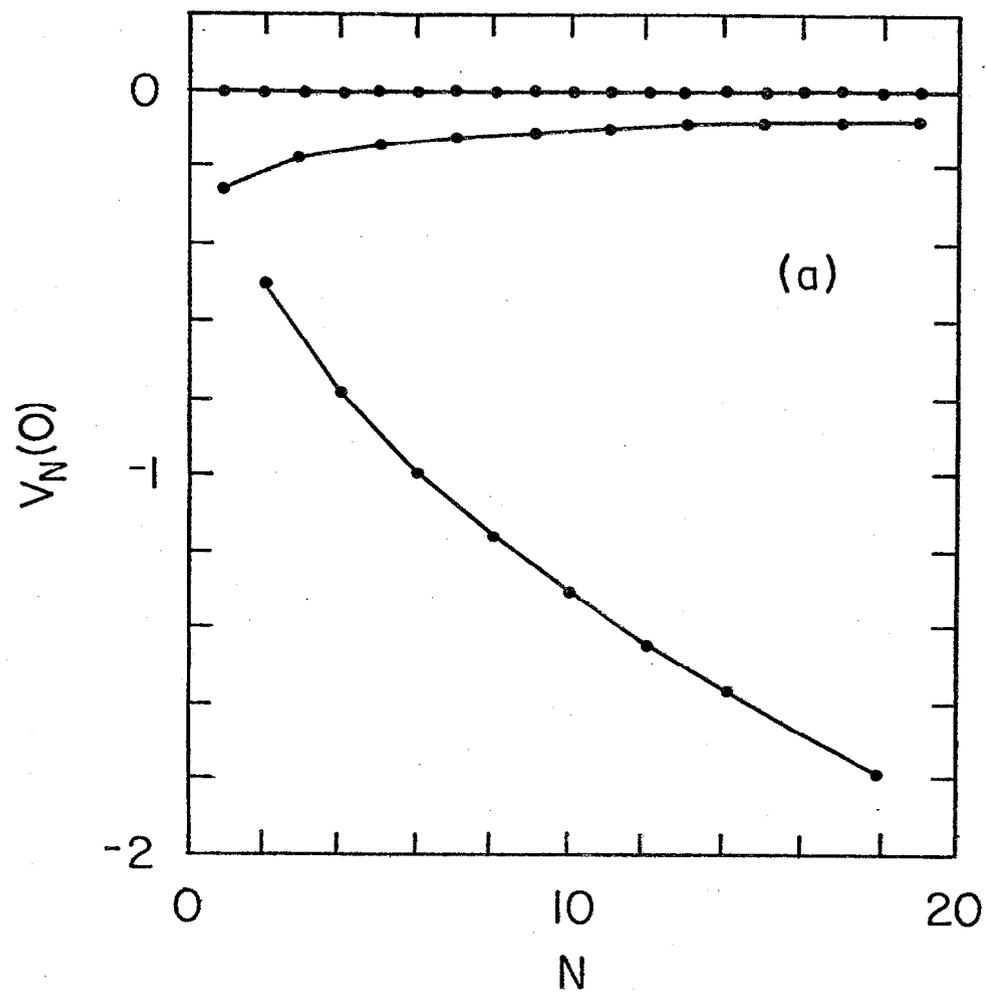


Fig. 5

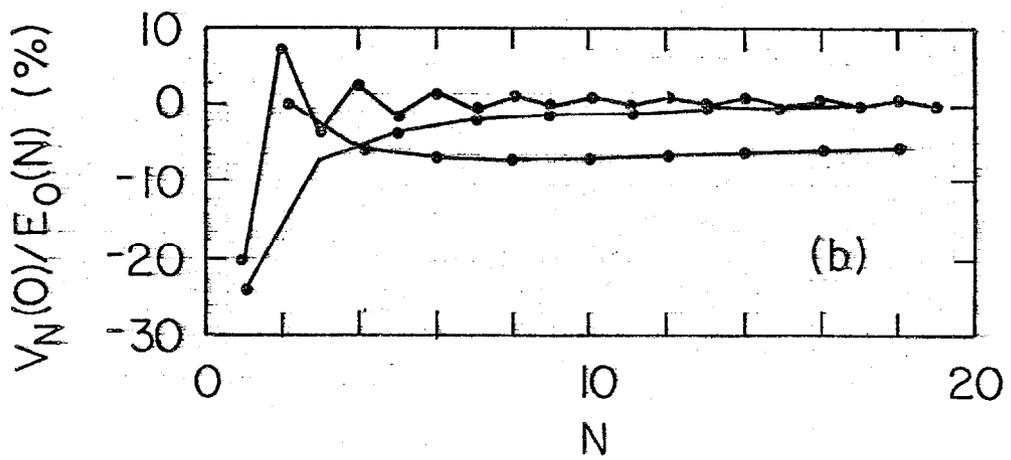
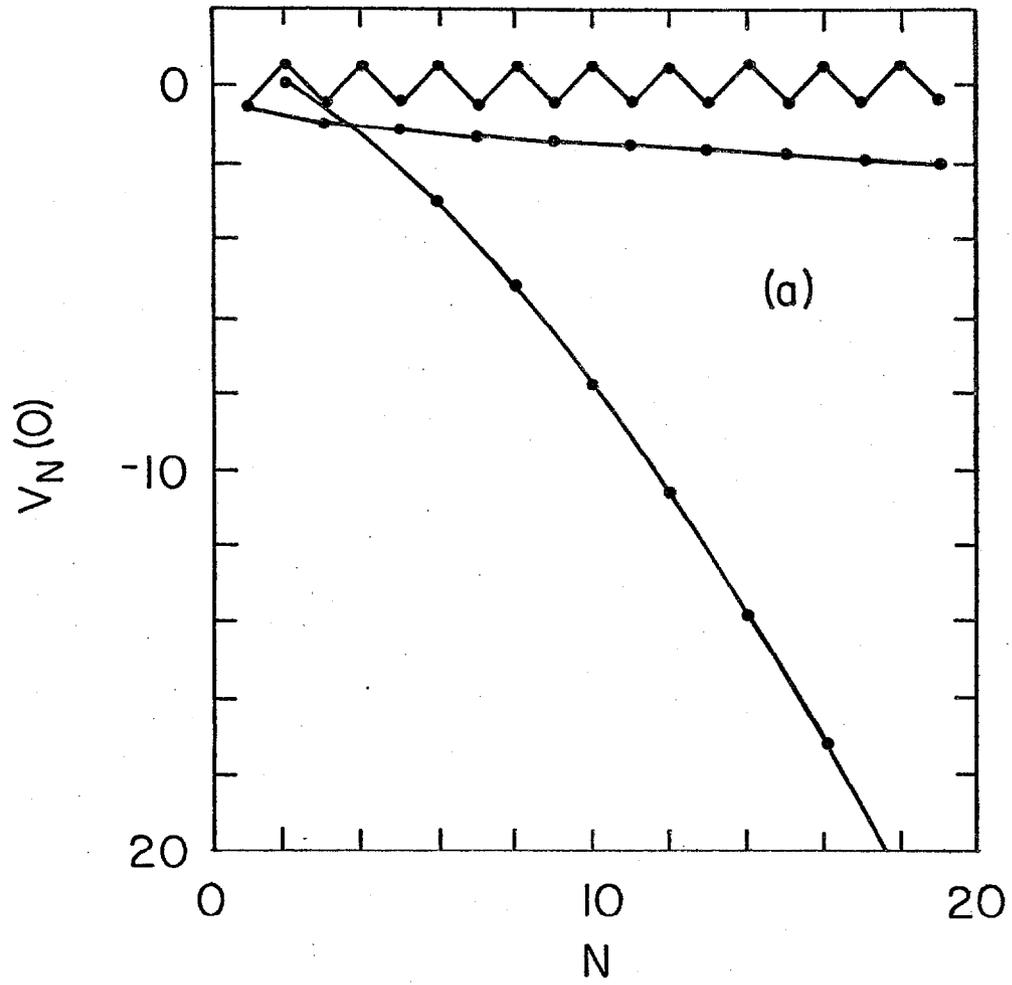


Fig. 6

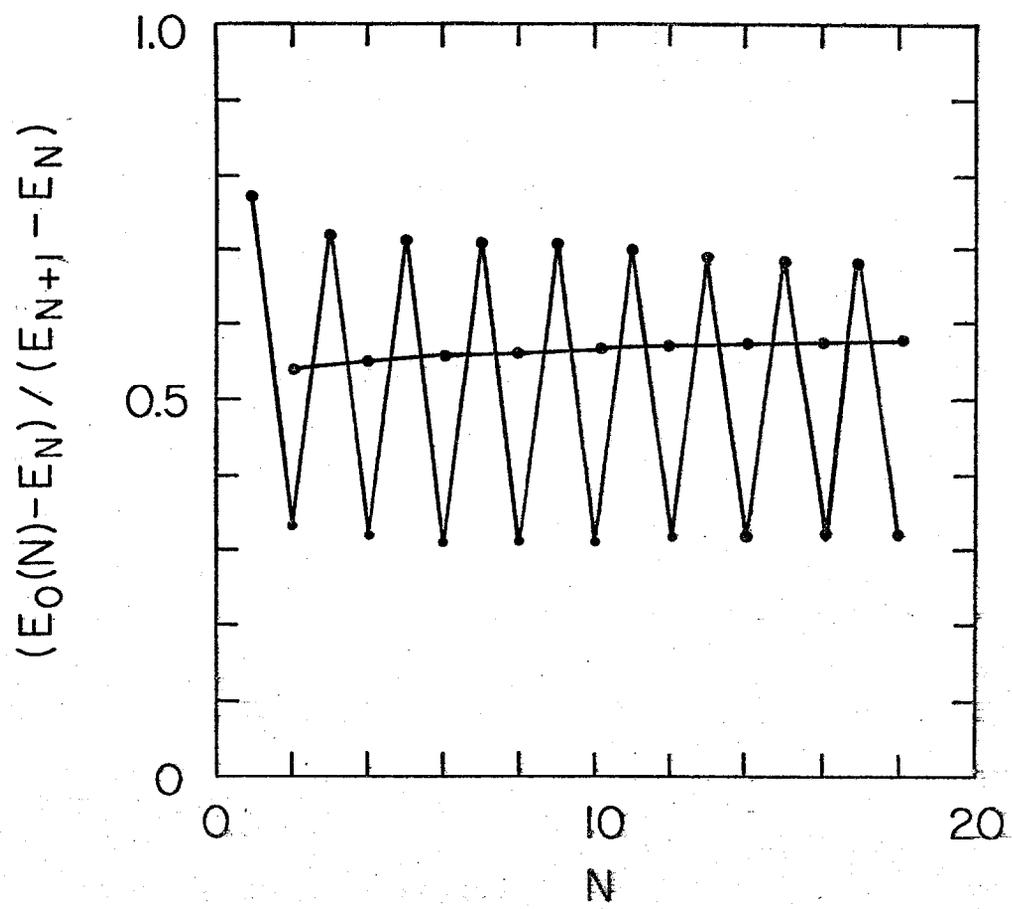


Fig. 7

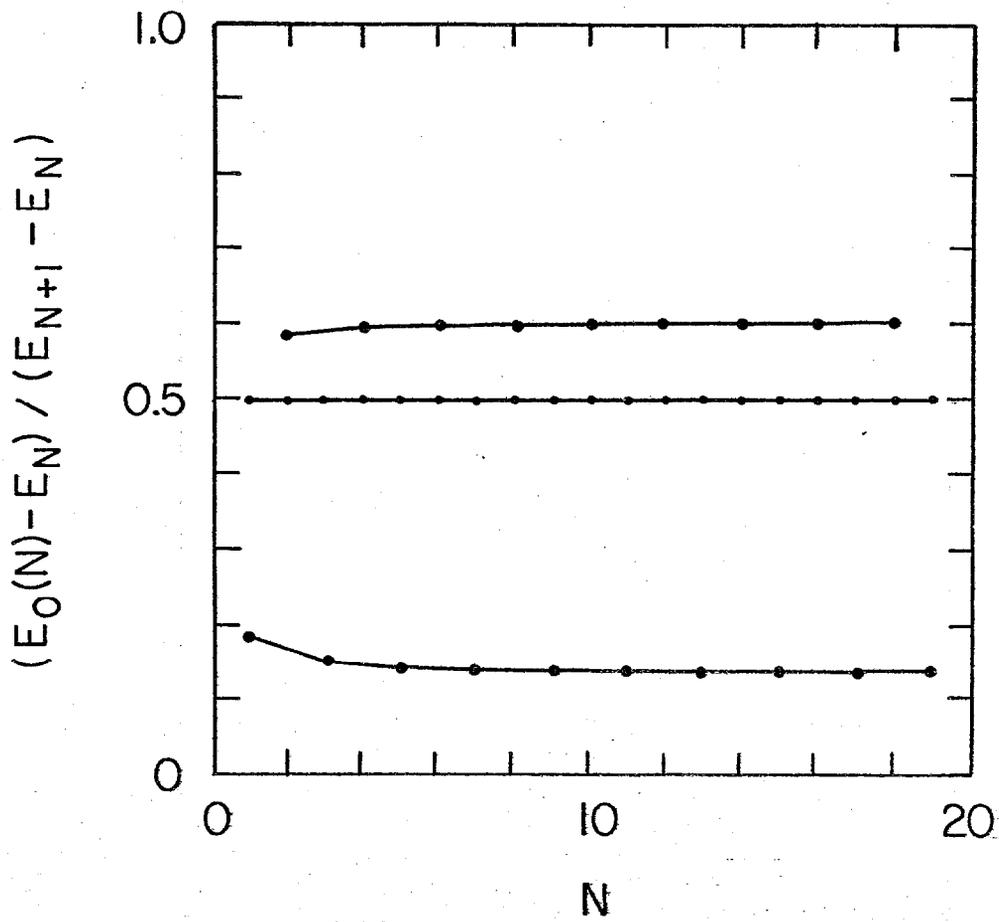


Fig. 8

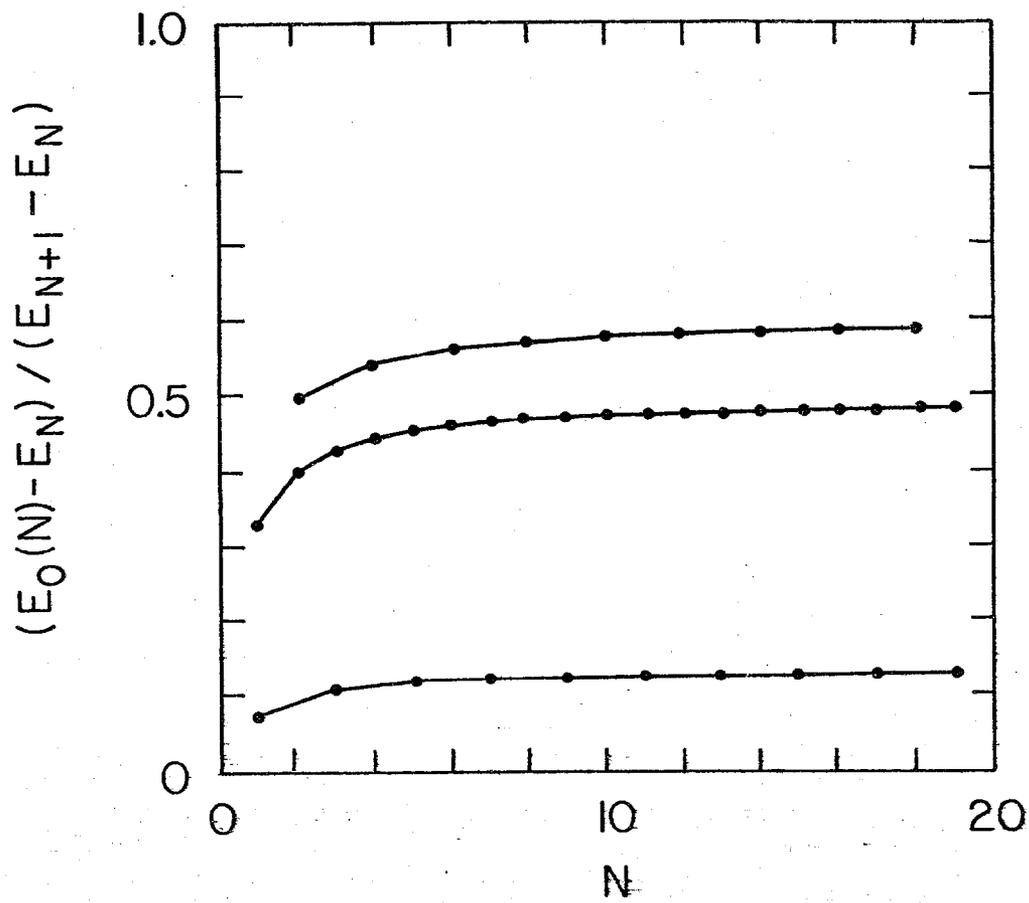


Fig. 9