PHYSICAL REVIEW A VOLUME 42, NUMBER 1 1 JULY 1990

Anomalies of the Schwinger variational phase shifts

Sadhan K. Adhikari
Departamento de Física, Universidade Federal de Pernambuco, 50.739 Recife, Pernambuco, Brazil
(Received 22 January 1990)

The origin of certain anomalies of the Schwinger variational phase shifts in momentum space is investigated. It is demonstrated that these anomalies are related to the appearance of continuum bound states in the approximate calculation.

I. INTRODUCTION

The Schwinger variational principle[1] has been extremely useful in the calculation of scattering phase shifts in a diverse class of quantum-mechanical problems.[2] The complete equivalence[3] between the method of separable expansion and the Schwinger variational principle has made the calculation of phase shifts using square-integrable basis functions a routine task.[2] In this method an operator involving the Green function is to be inverted and usually this procedure does not lead to spurious singularities[4] which are usually encountered[5] in calculations involving the Kohn variational principle[6] where the basis functions are to satisfy the asymptotic boundary condition of the physical wave functions.

Recently, Apagyi, Lévay, and Ladányi[7] have noted in their study of electron–hydrogen-atom scattering in the static exchange approximation that certain spurious singularities appear in the tangent of the singlet phase shifts computed by the Schwinger variational method in momentum space. Their triplet phase shifts, however, were free of these anomalies. The anomaly in the case of singlet scattering manifested itself in a sudden extra drop of the phase shift through π as energy is increased so that the phase-shift difference between 0 and ∞ energies $\delta(0)-\delta(\infty)$ increases by π under this situation. In a completely different context Haidenbauer and Plessas[8] found in their study of separable expansions of realistic nucleon-nucleon potentials that certain spurious anomalies appear in the triplet phase shifts computed in the ${}^3S_1-{}^3D_1$ channel. In particular, they found that the phase shift suddenly increases through π as energy is increased representing a resonancelike behavior. Both these anomalies apparently indicate a nearby pole of the t matrix. These anomalies together with the belief[4,9] that for local short-range potentials the Schwinger method is free of spurious singularities have led us to study the origin of these singularities. It is interesting to investigate whether these singularities are universal, i.e., independent of specific properties of the potential or the expansion functions, in nature or dependent on some specific properties of the potential or the expansion functions.

It is well known[3] that the Schwinger phase shifts are identical with those obtained from a rank-N separable potential V_N

$$V_N=\sum_{i,j=1}^{N} V|f_i\rangle C_{ij}\langle f_j|V\ , \tag{1.1}$$

where

$$(C^{-1})_{ji}=\langle f_j|V|f_i\rangle\ , \tag{1.2}$$

where $|f_i\rangle$, $i=i,2,\ldots,N$, are the L^2 expansion functions of the Schwinger method. The resultant t-matrix t_N is given by

$$t_N=\sum_{i,j=1}^{N} V|f_i\rangle D_{ij}\langle f_j|V\ , \tag{1.3}$$

where

$$(D^{-1})_{ji}=\langle f_j|(V-VG_0V)|f_i\rangle\ , \tag{1.4}$$

where $G_0\equiv(E-H_0+i0)^{-1}$ is the free-particle Green function, E is the parametric energy, and H_0 is the kinetic energy operator. A nonlocal potential, in general, and also the separable rank-N potential V_N, may sustain a continuum bound state[10] (CBS) at a positive energy. It is well known[10] that the appearance of such a CBS may lead to anomalies in the phase shifts calculated from t_N. In particular, we shall see that this may lead to a resonance-like jump of π in the phase shift when the CBS is nearby (as found in Ref. 8) and a drop of π in the phase shift when the CBS is on the real energy axis (as found in Ref. 7). From our study we find that the anomalies found in Refs. 7 and 8 are caused by a CBS. These anomalies are quite universal in nature and are not consequences of specific properties of the potential and expansion functions. Unless the expansion functions are also of definite sign, such anomalies, contrary to popular belief,[4,9] may appear even in the case of positive definite local short-range potentials. They do not appear for a positive definite local short-range potential if the expansion functions are also chosen to be of definite sign. We illustrate our conclusions by using a semiphenomenological nucleon-nucleon potential and a simple exponential expansion function.

In Sec. II we present a brief account of the CBS for a separable potential. In Sec. III we present a numerical investigation of anomalies for the Schwinger variational phase shifts. Finally, in Sec. IV we present some concluding remarks.

II. CONTINUUM BOUND STATE FOR SEPARABLE POTENTIALS

A nonlocal potential may possess a continuum bound state. The simplest example of a CBS is in a separable potential of rank 1. We illustrate some of the important features of the phase shift near a CBS. In the next section we report a numerical investigation of these properties in the case of a Schwinger variation calculation which uses a rank-one separable potential.

The on-shell t-matrix $t(k)$, $k^2=E$ in units $(\hbar^2/2m)=1$, where m is the reduced mass, parametrized as

$$t(k)=-\frac{e^{i\delta}\sin\delta}{k}\ , \tag{2.1}$$

can usually be written as

$$t(k)=\frac{N(k)}{D(k)}\ , \tag{2.2}$$

where $D(k)$ is the Fredholm determinant and possesses the unitarity cut and bound-state poles. The function $N(k)$ contains the left-hand singularities of the potential. Constraints of unitary require that $\mathrm{Im}D(k)=kN(k)$ and consequently

$$t(k)=\frac{N(k)}{\mathrm{Re}D(k)+ikN(k)}\ , \tag{2.3}$$

where Re and Im denote the real and imaginary parts, respectively.

At a CBS $D(k)=0$ and, consequently, $N(k)=0$. From Eqs. (2.1)–(2.3) it follows that at a CBS (Ref. 10) $\tan\delta$, given by

$$\tan\delta=-k\frac{N(k)}{\mathrm{Re}D(k)}\ , \tag{2.4}$$

becomes zero. The phase-shift δ drops through π as the energy k^2 increases through the CBS energy, which will lead to a modification of Levinson's theorem to[10]

$$\delta(0)-\delta(\infty)=(n+n')\pi\ , \tag{2.5}$$

where n is the number of bound states and n' is the number of CBS's.

A CBS corresponds to simultaneous zeros of $N(k)$ and $D(k)$ so that $\tan\delta$ of Eq. (2.4) is zero. If the potential parameters are slightly adjusted so that zeros of $N(k)$ and $D(k)$ are not simultaneous, the CBS disappears and moves into the complex energy plane. Then the nearby pole of the t matrix in the complex energy plane produces a resonancelike behavior and consequently, the phase shift jumps through π as the energy increases through this pole. Hence a nonlocal potential may produce a rapid variation in the phase shift due to the appearance of a CBS, which is not possible in the case of a local potential.

Next let us consider the problem of calculating the phase shifts of a local short-ranged potential using the Schwinger variational principle. It is well-known that this problem reduces to the evaluation of the t-matrix t_N of Eq. (1.3) for the rank-N separable potential V_N of Eq. (1.1). As the rank-N potential V_N is not local it may sustain a CBS and the phase shift so calculated may lead to spurious singularities discussed above for a specific choice of expansion functions.

We illustrate these in the case of the model nucleon-nucleon potential

$$V(r)=\sum_{j=1}^{2}V_j\frac{e^{-\mu_j r}}{r}\ , \tag{2.6}$$

where $V_1=-13.752\,87$ fm^{-1}, $\mu_1=1.55$ fm^{-1}, $V_2=34.687\,27$ fm^{-1}, $\mu_2=3.11$ fm^{-1}, cf. Eq. (34) of Ref. 3. We consider the expansion functions

$$f_n(r)=e^{-\alpha nr}\ , \tag{2.7}$$

in configuration space. In this case the t-matrix t_N of Eq. (1.3) is analytically calculable, cf. Eq. (30) of Ref. 3. For simplicity we consider the S-wave rank-one t matrix of the form (2.2) with

$$N(k)\equiv|\langle k|V|f_1\rangle|^2=\left|\sum_{j=1}^{2}\frac{V_j}{(\mu_j+\alpha)^2+k^2}\right|^2\ , \tag{2.8}$$

$$\begin{aligned}D(k)&\equiv\langle f_1|V-VG_0V)|f_1\rangle\\&=\sum_{j=1}^{2}\frac{V_j}{(\mu_j+2\alpha)^2}\\&\quad+\sum_{i,j=1}^{2}\frac{V_iV_j}{(2\alpha+\mu_i+\mu_j)(\alpha+\mu_i-ik)(\alpha+\mu_j-ik)}\ ,\end{aligned} \tag{2.9}$$

and the easily verified relation $\mathrm{Im}D(k)=kN(k)$. At a CBS both $N(k)$ and $D(k)$ should vanish. If both the potential $V(r)$ and the expansion function $f_1(r)$ are of definite sign $N(k)$ is not expected to vanish. If either $V(r)$ or $f_1(r)$ have an attractive and a repulsive part $N(k)$ can easily vanish and so can $D(k)$ leading to a CBS, which will lead to spurious singularities in the Schwinger variational phase shifts. The same thing should hold for a rank-N t-matrix t_N which may possess a CBS, though in the general rank-N case the expression for $N(k)$ and $D(k)$ can not be easily written down.

III. NUMERICAL INVESTIGATION

In this section we present results for phase-shift calculation of the potential (2.6) for the expansion function (2.7) with $n=1$. The reason for considering this model is that it is rich enough to exhibit all the anomalies of the Schwinger variational phase shifts yet simple enough to be manipulated in a controlled way and it is easy to identify the appearance of a CBS and the associated anomalies of the Schwinger variational phase shift.

The phase shift in this case is calculated via Eq. (2.1), (2.8), and (2.9). In this case the center-of-mass energy is given by $E=\hbar^2k^2/2m$, where m is the reduced mass of the nucleon-nucleon system, so that $\hbar^2/2m=41.47$ MeV fm^2. In this case we find that $N(k)$ has a zero for an E in the range $0<E<\infty$. The zero of $\mathrm{Re}D(k)$ coincides with that of $N(k)$ for $\alpha=0.14$ fm^{-1} signaling the appearance of a CBS at $E=92$ MeV.

We plot in Fig. 1 the phase shifts versus center-of-mass energies for various values of α. For $\alpha=0.14$ fm^{-1} there is a CBS at 92 MeV and consequently the phase shift

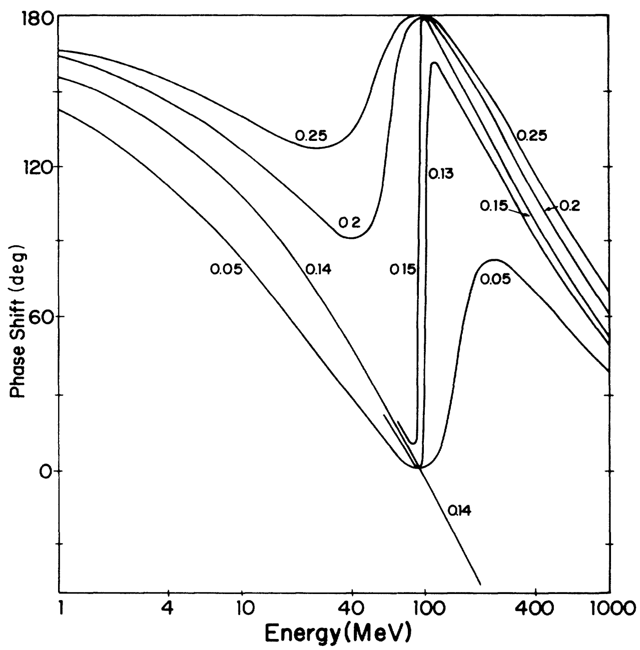

FIG. 1. Schwinger variational phase shifts for the potential (2.6) and expansion function $\exp(-\alpha r)$ vs energy E for various α. For $\alpha=0.14$ fm^{-1} we have the CBS at $E=92$ MeV and $\delta(\infty)$ goes to $-180°$ consistent with the modified Levinson's theorem: $\delta(0)-\delta(\infty)=2\pi$.

drops through π as the energy increases through the CBS energy. For α in the vicinity of 0.14 fm^{-1} the CBS moves into the complex energy plane and its effect on phase shift is like that of a resonance as is clear from the phase-shift curves for $\alpha=0.13$ and 0.15 fm^{-1}. In both cases the phase shift increases approximately through π as the energy increases through the spurious resonance energy. It is called spurious because the original potential (2.6) does not have any resonance. For $\alpha=0.14$ fm^{-1}, $\delta(0)-\delta(\infty)=2\pi$ according to the modified[10] Levinson theorem (2.5), as there is a real bound state and a CBS. For all other α's there is no CBS, at best there is a resonance and $\delta(0)-\delta(\infty)=\pi$.

The rank-1 model, despite possessing all these important features of the general rank-N model and of a general Schwinger variational calculation, has the limitation of producing phase shifts which are far from the converged result. For all α, $N(k)$ of Eq. (2.8) and hence $\tan\delta$ of Eq. (2.4) has a zero at a particular energy. Hence δ becomes either zero of π at this particular energy, which is clear from Fig. 1. This drawback is removed in a general rank-N $(N>1)$ model where δ does not need to be 0 or π between $E=0$ and ∞. This drawback does not, however, invalidate our conclusions.

Now it is easy to see that the anomaly observed by Apagyi *et al.* of the Schwinger phase shift (see Fig. 3 of Ref. 7) is due to a CBS for $N=5$ and $k\simeq 0.9$ a.u. The phase shift drops through π as k increases through this value. Consequently, Levinson's theorem has to be modified according to Eq. (2.5) in order to accommodate the CBS. The anomaly observed by Haidenbauer and Plessas (see Fig. 1 of Ref. 8) is due to a resonance for energy $E_L=300$ MeV. The phase shift jumps approximately through π as E_L increases past this value. The CBS in this case has moved into the complex energy plane and the usual Levinson's theorem holds in this case.

The potential (2.6) of the present study has a positive and a negative part; the expansion functions are, however, positive definite. This can make the form factors in Eq. (2.8) and consequently $D(k)$ vanish simultaneously at a particular k to make a CBS appear at this k, which leads to the anomaly we have studied. A CBS will not appear if the potential and the expansion functions are both chosen to be of definite sign. However, a CBS may appear in the case of a short-range potential of definite sign if the expansion functions are chosen to have a positive and a negative part.

IV. CONCLUSION

It is demonstrated that Schwinger variational phase shifts may present two types of anomalies. The first type is due to the appearance of a CBS at a positive energy, when the phase shift drops through π as the energy increases through this value. The second type appears when the CBS moves into the complex energy plane and behaves like a resonance. Then the phase shift increases sharply through π as energy increases through this value. These two types of anomalies were observed in Refs. 7 and 8, respectively, in the study of electron–hydrogen-atom and nucleon-nucleon scattering. We have demonstrated these anomalies in a simple Schwinger variational calculation which leads to a rank-one t matrix. This model allows one to vary the parameters of the expansion function in a simple and controlled way and allows one to interpret the anomalies in the Schwinger variational phase shifts easily. The conclusion about the anomalies are supposed to hold true in a more general context. These anomalies of the Schwinger variational phase shifts should be rare in practice and are expected to have little relevance to the usefulness of the Schwinger variational method, as has been pointed out recently.[11]

Finally, we should mention that the anomalies of the Schwinger variational phase shifts are of a different nature than those of the Kohn variational phase shifts. In the Kohn method one has to invert the operator $E-H$, where H is the full Hamiltonian. As H has continuum spectra at positive energies, unless the basis states of the Kohn method satisfying the scattering boundary condition are carefully chosen $(E-H)^{-1}$ may lead to spurious poles, which lead to the anomalies in the Kohn variational method.

ACKNOWLEDGMENTS

The work was supported in part by the Financiadora de Estudos e Projetos and Conselho Nacional de Desenvolvimento Científico e Tecnológico of Brazil.

[1]J. Schwinger, Phys. Rev. **72**, 742 (1947); **78**, 135 (1950); (unpublished).

[2]M. A. Abdel-Raouf, Phys. Rep. **108**, 1 (1984); J. Callaway, *ibid.* **45**, 89 (1978); R. R. Lucchese, K. Takatsuka, and V. Mckoy, *ibid.* **131**, 147 (1986).

[3]S. K. Adhikari and I. H. Sloan, Phys. Rev. C **11**, 1133 (1975).

[4]C. Schwartz, Phys. Rev. **141**, 1468 (1966).

[5]R. K. Nesbet, Phys. Rev. **175**, 134 (1968); R. K. Nesbet and J. D. Lyons, Phys. Rev. A **4**, 1812 (1971); D. G. Truhlar, J. Abdallah, and R. L. Smith, Adv. Chem. Phys. **25**, 211 (1974); M. A. Abdel-Raouf, Phys. Rev. A **30**, 2794 (1984).

[6]W. Kohn, Phys. Rev. **74**, 1763 (1948).

[7]B. Apagyi, P. Lévay, and K. Ladányi, Phys. Rev. A **37**, 4577 (1988).

[8]J. Haidenbauer and W. Plessas, Phys. Rev. C **27**, 63 (1983).

[9]T. Kato, Phys. Rev. **80**, 475 (1950); R. Sugar and R. Blankenbecler, *ibid.* **136**, 472 (1964).

[10]See, for example, B. Bagchi, T. O. Krause, and B. Mulligan, Phys. Rev. C **15**, 1623 (1977); B. Mulligan and S. B. Quadri, *ibid.* **24**, 874 (1981); L. L. Foldy, *ibid.* **28**, 1818 (1982).

[11]C. Winstead and V. McKoy, Phys. Rev. A **41**, 49 (1990).