# Application of the Schwinger Variational Principle for Scattering*

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The usual difficulty of having to evaluate double integrals with $G(x,x')$ is avoided by considering as the trial function $U(x)=V(x)\psi(x)$ and its Fourier transform. Numerical calculations of $s$-wave scattering by a Yukawa potential have been carried out both by means of this form of Schwinger's method and also by using Kohn's variational principle. For comparable trial functions, the latter method appears to converge faster.

FOR the Schrödinger equation

$$(E-H)\psi=0, \tag{1}$$

with the separation

$$H=H_0+V, \tag{2}$$

the conventional statements of formal scattering theory are:

$$\psi_a^{\pm}=\varphi_a+G^{\pm}V\psi_a^{\pm}, \tag{3}$$

$$G^{+}=1/(E-H_0+i\epsilon)=(G^{-})^{\dagger}, \tag{4}$$

$$(E-H_0)\varphi_a=0, \tag{5}$$

and the $T$-matrix elements are

$$T_{ba}=(\varphi_b,V\psi_a^{+})=(\psi_b^{-},V\varphi_a). \tag{6}$$

Schwinger's variational principle[1] gives

$$[T_{ba}]=(\varphi_b,V\psi_a^{+})+(\psi_b^{-},V\varphi_a)-(\psi_b^{-},V\psi_a^{+})+(\psi_b^{-},VG^{+}V\psi_a^{+}) \tag{7}$$

as a stationary expression for the $T$ matrix under arbitrary infinitesimal variations of the trial functions $\psi_a^{+}$ and $\psi_b^{-}$ about the exact solutions of (3). Although this variational principle has often been hailed as an elegant formulation of the scattering problem, only little use has been made of it as a practical computational tool.[2] The chief drawback stems from the fact that the Green's function is nonlocal in coordinate space, so that the last term in (7) requires the evaluation of the double integral

$$\int d\mathbf{x}\int d\mathbf{x}'\,\psi_b^{-*}(\mathbf{x}')V(\mathbf{x}')G^{+}(\mathbf{x}',\mathbf{x})V(\mathbf{x})\psi_a^{+}(\mathbf{x}). \tag{8}$$

We may compare this situation with that posed by the Kohn variational principle[3]:

$$[T_{ba}]=T_{ba}^{(\mathrm{trial})}-(\psi_b^{-},(E-H)\psi_a^{+}). \tag{9}$$

Here we have the advantage of the simpler local operator $(E-H)$, but the trial functions $\psi_a^{+},\psi_b^{-}$ must be constrained so that in the asymptotic region they have the correct form [as determined by (3)], with the only allowed variation taking place in the numbers $T_{ba}^{(\mathrm{trial})}$ associated with that form.

The purpose of the present paper is to describe a way of making the Schwinger form (7) more tractable. Instead of concentrating on $\psi(\mathbf{x})$ as the function to be varied, we define the new trial function

$$U(\mathbf{x})\equiv V(\mathbf{x})\psi(\mathbf{x}), \tag{10}$$

which we shall also need to represent, in momentum space

$$\tilde{U}(\mathbf{p})=\int d\mathbf{x}\,e^{-i\mathbf{p}\cdot\mathbf{x}}U(\mathbf{x}). \tag{11}$$

Assuming, as is generally the case, that the Green's function is diagonal in $p$ space,

$$G^{\pm}(\mathbf{x},\mathbf{x}')=\int\frac{d\mathbf{p}}{(2\pi)^3}e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}G^{\pm}(\mathbf{p}), \tag{12}$$

we can rewrite the Schwinger form as follows:

$$[T_{ba}]=\tilde{U}_a^{+}(\mathbf{k}_b)+\tilde{U}_b^{-*}(\mathbf{k}_a)-\int d\mathbf{x}\,U_b^{-*}(x)V^{-1}(x)U_a^{+}(x)+\int\frac{d\mathbf{p}}{(2\pi)^3}\tilde{U}_b^{-*}(\mathbf{p})G^{+}(\mathbf{p})\tilde{U}_a^{+}(\mathbf{p}). \tag{13}$$

In this form, we have to evaluate only *single* integrals: one in $x$ space, as befits $V$; and one in $p$ space, as befits $G$. A nice extra feature of this formulation is that $U(x)$ is a well-localized function—assuming $V(x)$ is—and one does not have to put plane-wave terms into this trial function, but can concentrate on the more interesting region of small $x$.

The novel feature of (13) is the appearance of the *inverse* of the potential. The reader may readily convince himself that this does not cause any serious difficulties; and, in fact, this is a very natural concomitance: the inverse of $V$ accompanying $G$, the inverse of $E-H_0$.

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[1] J. Schwinger, Harvard University, 1947 (unpublished).
[2] See, for example, the review article by H. S. W. Massey in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. 36, p. 265.
[3] W. Kohn, Phys. Rev. 74, 1763 (1948).

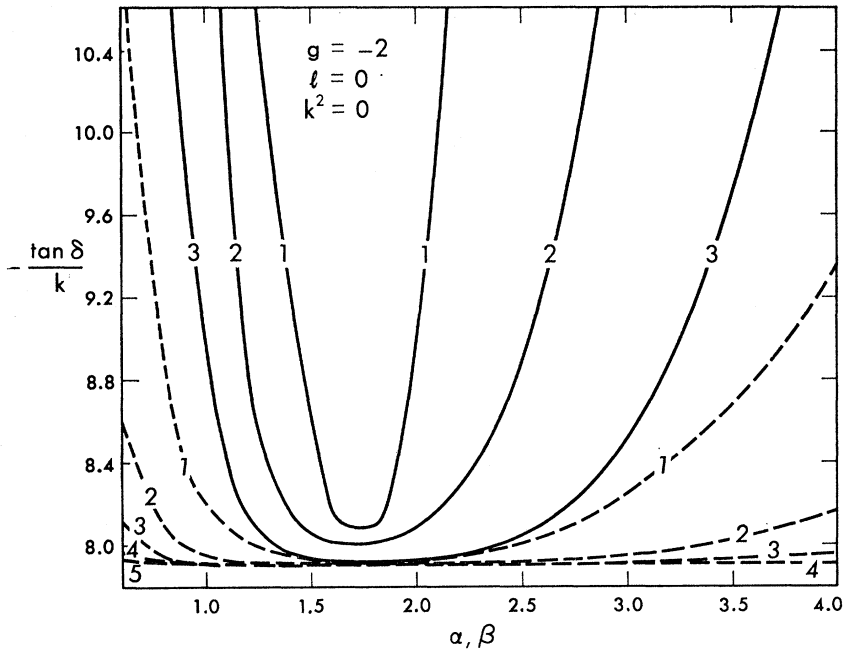


FIG. 1. Computed values of $-\tan\delta/k$ versus $\alpha$ or $\beta$ for Eq. (15) with $g=-2$, $k^2=0$. The solid curve is for the Schwinger method, the dotted curve for the Kohn method.

Further, our trial function $\tilde{U}_a(\mathbf{p})$ may be recognized as the $T$ matrix $T_{pa}$ with one leg off the energy shell. We can thus write our variational formulation (13) in the symbolic form (dropping all labels)

$$[T]=2T-TV^{-1}T+TGT, \tag{14}$$

with the advice that the $V$ term be evaluated in $x$ space and the $G$ term in $p$ space. Equation (14) emphasizes the fact that we have here a variational principle for the $T$ matrix itself, without any explicit reference to a wave function.

## SAMPLE CALCULATION

For a numerical exercise, we take the $s$-wave Schrödinger equation with a Yukawa potential:

$$\left(-\frac{1}{r}\frac{d^2}{dr^2}r+k^2\right)\psi=g\frac{e^{-r}}{r}\psi. \tag{15}$$

For our modified Schwinger method (13), we used the trial functions

$$\tilde{U}(p)=\sum_{n=1}^{N}\frac{C_n}{(p^2+\alpha^2)^n}, \tag{16}$$

which in $x$ space become

$$U(r)=-\frac{1}{r}\sum_{n=1}^{N}C_n'r^{n-1}e^{-\alpha r}. \tag{17}$$

For a comparative calculation with the Kohn method (9), we took the trial functions

$$\psi=\phi+\chi, \tag{18}$$

$$\phi=\frac{\sin kr}{kr}+\tan\delta^{(\text{trial})}\frac{\cos kr}{kr}(1-e^{-\beta r}), \tag{19}$$

$$\chi=\sum_{n=1}^{N}D_nr^{n-1}e^{-\beta r}. \tag{20}$$

Since $V\sim e^{-r}/r$, we see that, for appropriate choices of the scale parameters $\alpha$ and $\beta$, the wave functions represented by (17) and (20) span the same space. The Kohn trial function then appears to have the advantage of the explicit asymptotic terms represented by $\phi$. However, if there has ever been any virtue claimed for the Schwinger method, it is just that because it contains the Green's function explicitly, the asymptotic part of the wave function will be automatically taken care of. Therefore this appears to be a fair comparative test.

TABLE I. Successive approximations to the scattering length ($a=-\tan\delta/k$ at $k=0$) for the Yukawa potential of strength $g=-2$. Scale parameters $\alpha=\beta=1.8$.

| $N$ | $a$(Kohn) | $a$(Schwinger) |
|---|---|---|
| 1 | 7.92155 | 8.09387 |
| 2 | 7.91142 | 8.00863 |
| 3 | 7.91139 | 7.91228 |
| 4 | 7.91138 | 7.91178 |
| 5 | 7.91138 | 7.91178 |
| 6 | | 7.91147 |
| 7 | | 7.91142 |
| 8 | | 7.91139 |
| 9 | | 7.91138 |
| 10 | | 7.91138 |

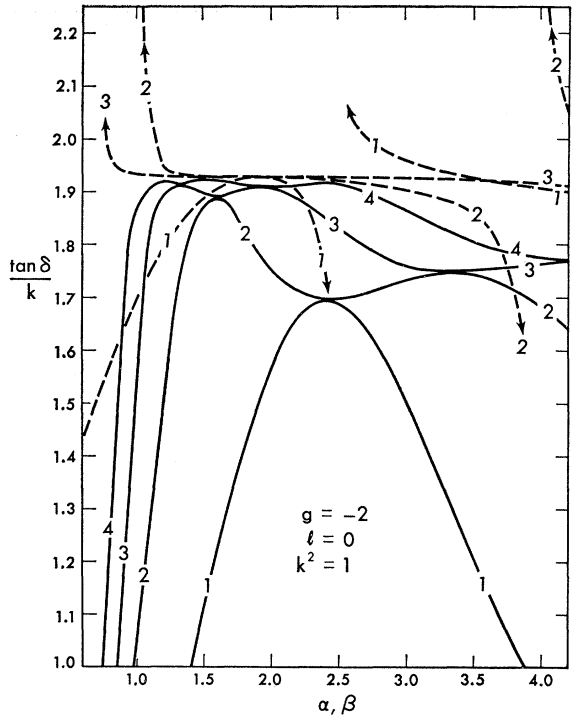


FIG. 2. Computed values of $\tan\delta/k$ versus $\alpha$ or $\beta$ for Eq. (15) with $g=-2$, $k^2=1$. The solid curve is for the Schwinger method, the dotted curve for the Kohn method.

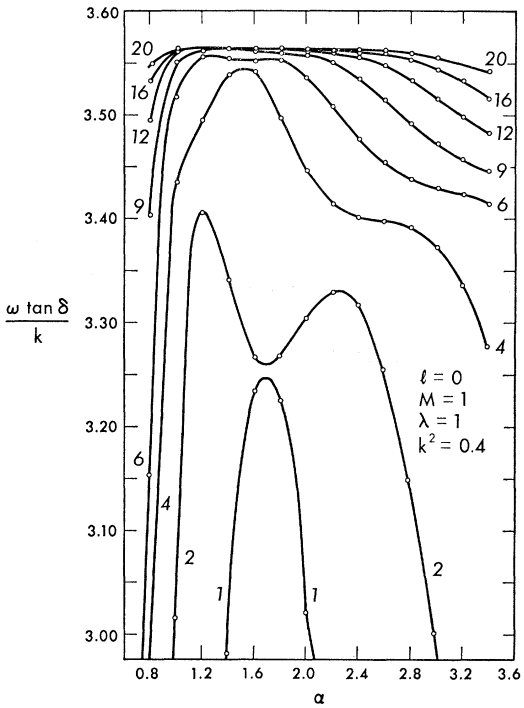


FIG. 3. Computed values of $(\omega/k)\tan\delta_0$ versus $\alpha$ for a Bethe-Salpeter equation (see Ref. 6), with $\lambda=1$, $M=1$, $k^2=0.4$. The curves are numbered to identify the number of basis functions used in the Schwinger variational method.

The integrals required by (13) were readily evaluated with the basis (16), (17); those needed for the Kohn method (9) were somewhat more tedious to grind out, mostly because of the extra $\phi$ terms. The entire numerical calculation was a quite trivial one on an electronic computer, and we now describe the results.

The stationary approximation to $\tan\delta/k$ was calculated for many values of the scale parameters $\alpha, \beta$ at several successive stages of approximation $N=1, 2, 3, \cdots$. Figure 1 shows the results at $k^2=0$ and $g=-2$ (the first bound $s$ state occurs at $g=-1.679809$). The values at $\alpha=\beta=1.8$ are listed in Table I for a finer comparison. Both methods obviously converge very nicely, but the Kohn method is clearly way ahead if one is greedy for accuracy.

In Fig. 2 are similar curves at a higher energy. Again the Kohn method is seen to converge much faster; but there is also more detail to talk about here. The Kohn-method curves show the occasional divergence which has been discussed previously[4]; and this phenomenon reduces somewhat the accuracy with which one can determine the true phase shifts. The Schwinger-method curves are free of this particular curse (the prediction to the contrary found in Ref. 4 is incorrect); the several curves are, in fact, prevented from crossing by the theorem[5] that for a potential everywhere attractive the Schwinger principle gives a lower bound for the phase shift. However, this apparent blessing may also cause some trouble. For suppose one calculated only at one fixed value of $\alpha$, such as $\alpha=2.4$ in Fig. 2; then one might draw quite a false conclusion about the accuracy of the second-order calculation, if one did not go on to higher approximations. Thus the curse of the Kohn method shows up in a rather different guise in the Schwinger method; and one must obey the general rule of getting a lot of information (such as Figs. 1, 2) before drawing quantitative conclusions about the accuracy of any variational calculations of scattering problems.

Other calculations, up to $k^2=16$, had the same general features described above.

In conclusion, we have seen that this form (13) of the Schwinger variational principle works very well as a practical computational method, although it appears that sometimes the Kohn method may still be more powerful. It is not clear if one can make further applications of this device to such other problems as many-body scattering. However, our new method has been used with great success in the solution of a Bethe-Salpeter equation,[6] where it turned out that a Kohn method was not usable. In Fig. 3 are curves, similar to those of Fig. 2, for that Bethe-Salpeter calculation. The resemblance is close enough so that we expect all the same general properties for that relativistic calculation, as for the nonrelativistic ones discussed in the present paper. Actually the Bethe-Salpeter results appear to converge at a faster rate for the cases illustrated here.

[4] C. Schwartz, Ann. Phys. (N. Y.) **16**, 36 (1961).
[5] T. Kato, Phys. Rev. **80**, 475 (1950); extended by R. Sugar and R. Blankenbecler, *ibid.* **136**, B472 (1964).
[6] C. Schwartz and C. Zemach, preceding paper, Phys. Rev. **141**, 1454 (1966).