Parametric equations of motion for the transition operator and the Green's operator

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An approach based on parametric equations of motion for the transition operator and the Green's operator is presented. The formulation applies generally to discrete and continuous states of quantum-mechanical many-body systems. The method provides an alternative to solving the Schrödinger equation as a boundary value problem by replacing it with an equivalent initial value problem.

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It has long been recognized that directly solving the Schrödinger equation for quantum-mechanical many-body systems can be prohibitively difficult and alternatives aiming at simplifying these procedures are desirable. Conventional methods, in general, deal with the Schrödinger equation as a boundary value problem either explicitly or implicitly. For bound state systems, Pechukas [1] proposed a different approach by treating Planck's constant $\hbar$ as a parameter, thereby converting the Schrödinger equation into a parametric equation of motion (PEM) with respect to $\hbar$ to be solved as an initial value problem. This approach has been employed to investigate quantum chaos [2–4] eigenvalues and eigenvectors of bound quantum systems [5,6], molecular potentials [7], and the dependence of photodynamics on different field parameters [8,9]. These earlier PEMs have, however, focused on the treatment of bound states, and, to the best of our knowledge, there has been no effort to derive a PEM for continuous states. In this paper, we present a more comprehensive PEM approach to a general quantum many-body system for both discrete bound states and continuous scattering states. We derive PEMs for physically important quantities, the transition operator, and the Green's operator and show that these PEMs can successfully replace the numerically difficult boundary value problem with an equivalent initial value problem.

For a Hamiltonian,

$$H_\lambda = H_0 + \lambda V, \tag{1}$$

where H_0 and V are independent of λ, the Lippmann-Schwinger equation for the transition operator T is given by

$$T_\lambda(E^+) = \lambda V + \lambda V G_0(E^+) T_\lambda(E^+), \tag{2}$$

where $G_0(E^+) = (E - H_0 + i\epsilon)^{-1}$. Taking the derivative with respect to λ on both sides of Eq. (2) and performing some operator algebra, we obtain the PEM for the transition operator,

$$\frac{dT_\lambda(E^+)}{d\lambda} = \frac{1}{\lambda}[T_\lambda(E^+) + T_\lambda(E^+) G_0(E^+) T_\lambda(E^+)] \tag{3}$$

with the initial conditions

$$T_0(E^+) = 0 \quad \text{and} \quad \left.\frac{dT_\lambda(E^+)}{d\lambda}\right|_{\lambda=0} = V. \tag{4}$$

Equation (3) may be solved by propagating λ from 0 to 1 using standard techniques for integrating ordinary differential equations. This PEM for the transition operator is entirely general and can be applied in principle to any many-body system. It is particularly appealing to use it for determination of transition matrices whose wave vectors are off the energy shell since the solution of PEM automatically contains all the matrix elements.

The coupling of the transition operator and the Green's function in Eq. (3) requires integration over the entire momentum space. Numerically, this can be very demanding since the T matrix generally oscillates rapidly as the length of the wave vectors and/or the incident energy increases, and its amplitude vanishes very slowly in the asymptotic region (roughly, inversely proportional to the length of the wave vector). Here we derive an alternative approach to obtain the T matrix by further developing a PEM for the Green's operator. Differentiating the equation

$$G_\lambda(E^+) = G_0(E^+) + G_0(E^+) T_\lambda(E^+) G_0(E^+), \tag{5}$$

we have

$$\frac{dG_\lambda(E^+)}{d\lambda} = G_0(E^+) \frac{dT_\lambda(E^+)}{d\lambda} G_0(E^+). \tag{6}$$

Substitution of Eq. (3) into Eq. (6) yields

$$\frac{dG_\lambda(E^+)}{d\lambda} = G_\lambda(E^+) V G_\lambda(E^+). \tag{7}$$

Equation (7) is the PEM for the Green's operator. A numerical implementation of this equation can be readily carried out. Unlike the case of the T-matrix PEM, it does not involve principal value integration arising from the Green's operator G_0. Because the potential function V vanishes rapidly as the interparticle distance increases, the PEM for G offers better numerical stability.

The utility of the PEM approach may be easily demonstrated using an example. Since the goal of this approach is to replace the numerically difficult boundary value scattering

problem by an initial value problem, we consider T-matrix elements in a square-integrable (L^2) basis set. This is not a requirement of the PEM approach, but it does allow the usual asymptotic matching procedures to be avoided. The PEM for the $\boldsymbol{T}$-matrix elements is

$$\frac{d}{d\lambda}\langle\phi_i|T_\lambda|\phi_j\rangle=\frac{1}{\lambda}\left[\langle\phi_i|T_\lambda|\phi_j\rangle+\sum_{k,l}\langle\phi_i|T_\lambda|\phi_k\rangle G_{k,l}(E^+)\times\langle\phi_i|\boldsymbol{T}_\lambda|\phi_j\rangle\right], \tag{8}$$

where ϕ_i is an L^2 basis function and $G_{k,l}(E^+)$ is the matrix representation of the outgoing wave Green's operator $\boldsymbol{G_0}$ in the L^2 basis set. It is convenient to define

$$G_{k,l}(E^+)=G_{k,l}(E)-iF_{k,l}(E), \tag{9}$$

$$G_{k,l}(E)=\sum_m\frac{\langle\phi_k|\theta_m\rangle\langle\theta_m|\phi_l\rangle}{E-E_m},$$
$$F_{k,l}(E)=\pi\frac{\langle\phi_k|\theta_E\rangle\langle\theta_E|\phi_l\rangle}{w_E}. \tag{10}$$

In the matrix representation used above, θ_m and E_m denote the mth eigenfunction and eigenvalue of $\boldsymbol{H_0}$, and w_E is an equivalent quadrature weight [10] that provides an energy renormalization of the unit-normalized matrix eigenfunction. The notation θ_E indicates that an interpolation of the matrix eigenfunction has been performed and evaluated at the energy E. The on-shell T-matrix element and cross section are given by

$$\langle E|T_\lambda|E\rangle=\sum_{i,j}F_{i,j}(E)\langle\phi_i|T_\lambda|\phi_j\rangle, \tag{11}$$

$$\sigma=\frac{4\pi}{k^2}|\langle E|T_\lambda|E\rangle|^2. \tag{12}$$

A mathematically equivalent but numerically more efficient approach is obtained using Eq. (7). The PEM for the G-matrix elements is

$$\frac{d}{d\lambda}\langle\phi_i|G_\lambda|\phi_j\rangle=\sum_{k,l}\langle\phi_i|G_\lambda|\phi_k\rangle\langle\phi_k|V|\phi_l\rangle\langle\phi_l|G_\lambda|\phi_j\rangle \tag{13}$$

with the initial condition $\boldsymbol{G_0}$ given by Eq. (9). The desired $\boldsymbol{T}$-matrix element is given by Eq. (11) using the solution to Eq. (13) and the identity

$$\langle\phi_i|\boldsymbol{T}_\lambda|\phi_j\rangle=\langle\phi_i|V|\phi_j\rangle+\sum_{k,l}\langle\phi_i|V|\phi_k\rangle\langle\phi_k|G_\lambda|\phi_l\rangle\times\langle\phi_l|V|\phi_j\rangle. \tag{14}$$

It is worth noting that although the first term in Eq. (14) is identical to the leading-order term of a perturbative Born series, the PEM formulation is nonperturbative. In fact, this is one of the strengths of the method in that it may be applied to problems where perturbation theory breaks down. To see this, we solve the PEMs for the $\boldsymbol{G}$-matrix and $\boldsymbol{T}$-matrix elements over a wide range of energies using a Laguerre polynomial basis set and a potential energy function of the form

$$V(r)=C\left(\frac{e^{-r}}{r^n}\right). \tag{15}$$

The code was tested for zero angular momentum using an exponential potential ($n=0$) and a Yukawa potential ($n=1$). The cross sections are shown in Figs. 1–3 as a function of wave number k. Each calculation used 40 basis functions. The PEM results for the $\boldsymbol{G}$-matrix method were identical to those for the T-matrix method. The $\boldsymbol{G}$-matrix method, however, was significantly more efficient in propagating over λ (see the discussion above). The "exact" results shown on

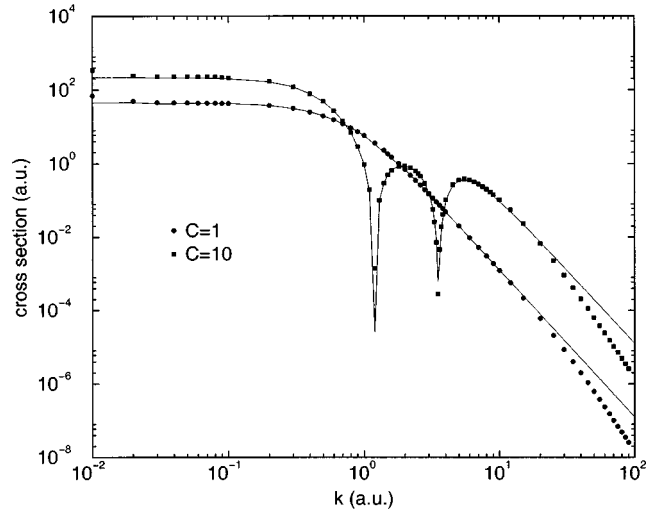

FIG. 1. Cross section as a function of k for an exponential potential ($n=0$). The solid lines are the "exact" results computed by numerical integration of the Schrödinger equation.

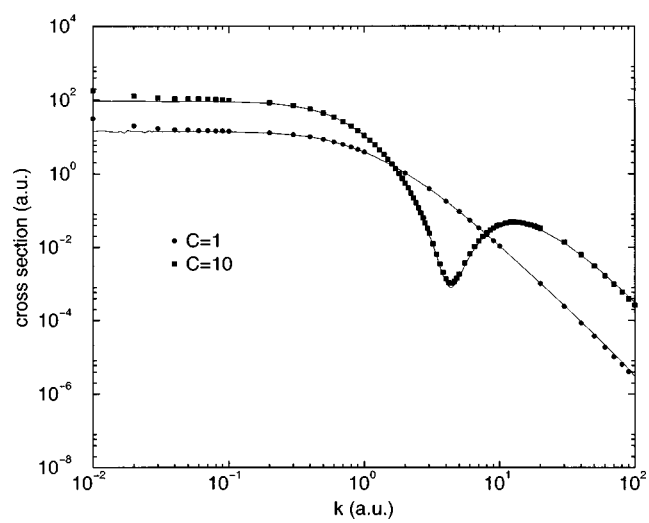

FIG. 2. Cross section as a function of k for a Yukawa potential ($n=1$). The solid lines are the "exact" results computed by numerical integration of the Schrödinger equation.

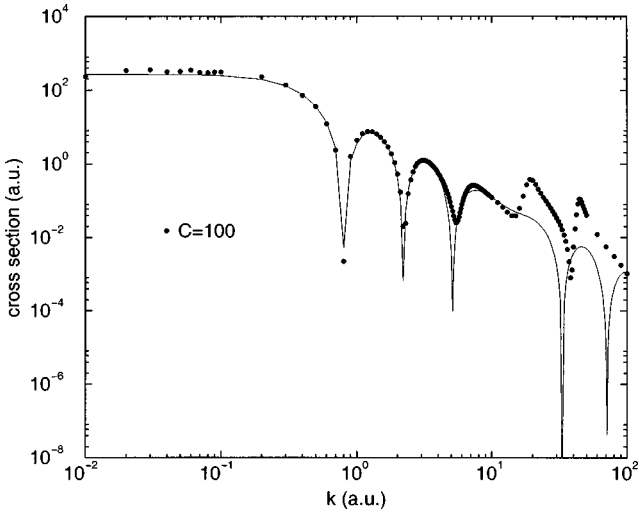

FIG. 3. Cross section as a function of k for a Yukawa potential ($n=1$). The solid line is the "exact" results computed by numerical integration of the Schrödinger equation.

the graphs were computed by numerical integration of the Schrödinger equation. The figures show that the PEM results are well-converged for most values of k. The convergence is slower at very low wave numbers and at very high wave numbers. At the very low wave numbers where Wigner threshold laws apply, more basis functions are needed to adequately represent the wave function at large distances. At very high wave numbers, the Laguerre polynomial basis set has difficulty representing the many oscillations that occur at such high energies. In this case, however, the contribution from the second term in Eq. (14) is negligible and the slow convergence is unrelated to the PEM formulation. Figure 3 shows that the convergence rate also decreases as the potential coupling is increased, particularly at high energies. These results suggest that the choice of basis set is an important consideration when applying the PEMs to a particular problem and that further investigation is needed. Nevertheless, the results clearly demonstrate that the PEMs provide a numerically stable foundation for computing the properties of quantum-mechanical systems.

In summary, we have obtained the PEMs for the transition operator and the Green's operator for many-body systems. PEMs for other quantities, such as the scattering operator and wave function, can be readily derived in a similar way using the PEM for the Green's operator. We tested the numerical properties of the PEMs using a square-integrable basis set and a model potential-energy function. The unique advantage of the PEM approach is that it allows full quantum-mechanical calculations using standard numerical techniques for solving initial value ordinary differential equations. The PEMs thus offer an alternative to the conventional quantum-mechanical methods for calculation of physical quantities, which would otherwise require that the Schrödinger equation be solved directly. The evaluation of the transition matrix may be conveniently performed for the entire energy spectrum regardless of being on or off the energy shell. Calculation of the Green's functions for both discrete and continuous quantum states may also be performed easily by taking advantage of the narrow range of most potential functions which vanish at sufficiently large interparticle separations.

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