

Applications of nonequilibrium Green functions to time-dependent decaying systems

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We used nonequilibrium many-body Green techniques for the time varying resonant phenomena in few-body systems. By relating the transition energy shift and width to the self-energy and by applying the functional variational techniques to the transition energy shift and width, the corresponding initial state resonant wave functions are derived. Then we obtained time-dependent decaying state wave functions, evolving from these initial states by solving the time-dependent Schrödinger equation for the decaying system numerically. Finally, we observed the plausible time decaying behaviors of our model as predicted by real few-body systems.

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When we investigate multichannel scattering, we use one of several different methods including distorted wave approximation, close coupling methods, and S -matrix and R -matrix methods [1,2]. However, when we consider quasi-bound states of the decaying processes, the above-mentioned procedures are generally very complex to apply. Complex coordinate techniques [3–9] have been developed for this purpose which are simpler than the above-mentioned standard procedures, especially in the neighborhood of the resonant energy ranges. Recently nonequilibrium Green function methods [10] have been attempted for the noncollective resonant processes of the model potential of δ barrier to evaluate the resonance parameters [11].

In this Brief Report we apply these techniques to the same model for the study of time-dependent behavior of the decaying system. For this purpose, we consider a few particle system. However, when field quantization is applied, this system is reduced to a corresponding single particle resonance scattering system with bound states by introducing a hypothetical model potential. Let $\psi_\alpha(\mathbf{r})$ be the initial wave functions of decaying states. These states can be represented using decaying state annihilation and creation operators \hat{F}_α and \hat{F}_α^\dagger , respectively. The bound state operators $\hat{\mu}_\alpha$ and $\hat{\mu}_\alpha^\dagger$, respectively, satisfy Bose commutation relations, $[\hat{\mu}_\alpha, \hat{\mu}_\beta] = 0$ and $[\hat{\mu}_\alpha, \hat{\mu}_\beta^\dagger] = \delta_{\alpha\beta}$. We now try to find a unitary transformation \hat{O} which shifts the description of decaying states to the bound state operators. The creation and annihilation operators for the α th decaying state of quantum mechanical one particle system are

$$\hat{F}_\alpha^\dagger = \int d\mathbf{r} \psi_\alpha(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \quad \text{and} \quad \hat{F}_\alpha = \int d\mathbf{r} \psi_\alpha^*(\mathbf{r}) \hat{\psi}(\mathbf{r}),$$

where the field operators satisfy the Bose commutation relations. Then we define a unitary operator,

$$\hat{O}(\varepsilon) = \exp(\varepsilon \hat{B}),$$

where $\hat{B} = \sum_\alpha (\hat{F}_\alpha^\dagger \hat{\mu}_\alpha - \hat{\mu}_\alpha^\dagger \hat{F}_\alpha)$ is an anti-Hermitian operator and ε is a real number to be determined. If we let $\hat{\mu}_\alpha(\varepsilon)$ be the transformed operator of an arbitrary operator of $\hat{\mu}_\alpha$, then after some manipulation for the derivative of the transformed bound operator, the derivative of the transformed decaying

state operator, and using the initial conditions $\hat{\mu}_\alpha(0) = \hat{\mu}_\alpha$ and $\hat{\mu}_\alpha'(0) = -\hat{F}_\alpha$, we obtain

$$\hat{\mu}_\alpha(\varepsilon) = \hat{\mu}_\alpha \cos \varepsilon - \hat{F}_\alpha \sin \varepsilon.$$

Let \hat{O} be the transformation for $\varepsilon = \pi/2$, $\psi_{\mathbf{k}}(\mathbf{r})$ the normalized free particle wave function with wave vector \mathbf{k} , and $\hat{\mu}_{\mathbf{k}}$, $\hat{\mu}_{\mathbf{k}}^\dagger$ the free particle annihilation and creation operators, respectively. Then using the transformed field operator and after some arrangement, we finally derive the Tani Hamiltonian which takes the bound states explicitly into consideration [11].

Next, using Liouvillian operator \hat{L} , \hat{F}_α satisfies the Heisenberg equations of motion,

$$i \frac{\partial \hat{F}_\alpha(t)}{\partial t} = [\hat{F}_\alpha(t), \hat{H}] = \hat{L} \hat{F}_\alpha(t). \quad (1)$$

In this paper the usual traditional algebraic procedure is employed. Hence the Liouvillian Green function is finally expressed in terms of expectation values (in terms of real numbers) of decaying state operators,

$$G(\alpha, t | \alpha, 0) = -i \langle \hat{F}_\alpha(t) \hat{F}_\alpha^\dagger \rangle, \quad t \geq 0,$$

where

$$\langle \hat{F}_\alpha(t) \hat{F}_\alpha^\dagger \rangle = \langle e^{i\hat{H}t} \hat{F}_\alpha e^{-i\hat{H}t} \hat{F}_\alpha^\dagger \rangle = \langle \hat{F}_\alpha e^{-i\hat{H}t} \hat{F}_\alpha^\dagger \rangle.$$

Hence the Liouvillian Green function is related to the persistence amplitude which is the probability of finding the same energy state ψ_α at time t . There exists some linearly independent operator basis such that the evolution of $\hat{F}_\alpha(t)$ may be expanded in terms of this basis,

$$\hat{L} \hat{F}_\alpha = [\hat{F}_\alpha, \hat{H}] = \sum_n \gamma(\alpha | n) \hat{\tau}_n, \quad (2)$$

where $\gamma(\alpha | n)$ are the complete matrix elements of the Liouvillian operators with respect to the operator basis $\hat{\tau}_n$. From Eqs. (1) and (2), and using the Laplace transformation, we obtain transformed Green function, $\tilde{G}(\alpha, z | \alpha, 0)$.

Let us assume that Green function $\tilde{G}(\alpha, t | \alpha, 0)$ increases less rapidly than exponentially as t approaches $+\infty$; then the Laplace transforms of $\tilde{G}(\alpha, z | \alpha, 0)$ will be analytic in the

upper half complex energy plane. For a decaying system the analytical continuation of $\tilde{G}(\alpha, z|\alpha, 0)$ into the lower half complex energy plane will have a complex pole z_α , which becomes u_α as the interaction vanishes. From the analytic behavior of $\tilde{G}(\alpha, z|\alpha, 0)$ we can propose the following form of Green functions:

$$\tilde{G}(\alpha, z|\alpha, 0) = \frac{iG(\alpha, 0|\alpha, 0)}{z - u_\alpha - \Sigma_\alpha(z)},$$

where $\Sigma_\alpha(z)$ will be called the self-energy. Then after rearrangement we derive the self-energy through the second order [10],

$$\sum_\alpha^{(2)}(z) = \int d\mathbf{k} \frac{\gamma(\alpha|\mathbf{k})\gamma(\mathbf{k}|n)}{u_\alpha - 1/2k^2 + i\eta}.$$

By introducing function $\zeta(\mathbf{r})$ such that the above formula can be represented in more practical form [10],

$$\begin{aligned} \sum_\alpha^{(2)}(z) = & - \int d\mathbf{r} \psi_\alpha^*(\mathbf{r})[H(\mathbf{r}) - u_\alpha]\psi_\alpha(\mathbf{r}) \\ & - \int d\mathbf{r} \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})\psi_\alpha(\mathbf{r}) \\ & + \int d\mathbf{r} \int d\mathbf{r}' \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})G_\alpha(\mathbf{r}, \mathbf{r}')\zeta(\mathbf{r}')\psi_\alpha(\mathbf{r}') \end{aligned} \quad (3)$$

where

$$G_\alpha(\mathbf{r}, \mathbf{r}') = \int d\mathbf{k} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{(2\pi)^3(u_\alpha - \frac{1}{2}k^2)}.$$

The variation process is related to the least variation of trial functions. If we extend this stabilization process to the exact variational method with the functional derivative, we suggest that the solutions obtained from this variational process corresponds to the resonance poles for a decaying system.

For our decaying system the functional is a complex valued function of decaying state waves, $\psi_\alpha(\mathbf{r})$ and $\psi_\alpha^*(\mathbf{r})$,

$$z_\alpha - \lambda_\alpha(\psi_\alpha, \psi_\alpha) = u_\alpha + \Delta_\alpha^{(2)} - i\eta_\alpha^{(2)} - \lambda_\alpha(\psi_\alpha, \psi_\alpha),$$

where λ_α are Lagrange undetermined coefficients due to the normalization of the resonance wave functions and $(\psi_\alpha, \psi_\alpha)$ is the inner product of trial α th decaying state wave functions. In this respect our decaying state wave functions are different from Gamow-Siegert states which are non-normalizable outgoing waves. Using Eq. (3),

$$\begin{aligned} z_\alpha - \lambda_\alpha(\psi_\alpha, \psi_\alpha) = & \int d\mathbf{r} \psi_\alpha^*(\mathbf{r})H(\mathbf{r})\psi_\alpha(\mathbf{r}) \\ & - \int d\mathbf{r} \psi_\alpha^*(\mathbf{r})[H(\mathbf{r}) - u_\alpha]\psi_\alpha(\mathbf{r}) \\ & - \int d\mathbf{r} \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})\psi_\alpha(\mathbf{r}) \\ & + \int d\mathbf{r} \int d\mathbf{r}' \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})G_\alpha(\mathbf{r}, \mathbf{r}') \end{aligned}$$

$$\times \zeta(\mathbf{r}')\psi_\alpha(\mathbf{r}') - \lambda_\alpha(\psi_\alpha, \psi_\alpha).$$

Now we define the functional derivative

$$\frac{\delta F[\psi]}{\delta \psi(\chi')} = \lim_{\lambda \rightarrow 0} \frac{1}{\lambda} \delta F[\psi], \quad (4)$$

where $\delta F[\psi] = F[\psi(\chi) + \lambda \delta(\chi - \chi')] - F[\psi]$. With atomic units, $m = \hbar = e = 1$ and by letting

$$\kappa = \int d\mathbf{r} \int d\mathbf{r}' \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r}) \frac{\delta G_\alpha(\mathbf{r}, \mathbf{r}')}{\delta u_\alpha} \zeta(\mathbf{r}')\psi_\alpha(\mathbf{r}'),$$

$$\xi(\mathbf{r}) = \int d\mathbf{r}' G_\alpha(\mathbf{r}, \mathbf{r}')\zeta(\mathbf{r}')\psi_\alpha(\mathbf{r}'),$$

Eq. (4) will be finally written as

$$-\frac{(1+\kappa)}{2} \nabla^2 \psi_\alpha(\mathbf{r}) + \zeta(\mathbf{r})\kappa\psi_\alpha(\mathbf{r}) + \zeta(\mathbf{r})\xi(\mathbf{r}) = (\lambda_\alpha - u_\alpha)\psi_\alpha(\mathbf{r}).$$

We now apply the variational method to our model, δ shell potential. This potential can roughly be regarded as a model potential for a particle tunneling out of a self-field created by a metastable excited resonant atom. By considering a single spinless boson particle tunneling out of the potential, $b\delta(r-a)$, where a, b are positive real numbers, we evaluate the S -state wave functions, $\psi_\alpha(r)$ [11].

In order to derive the time-dependent resonant phenomena, we recognize the time-dependent phenomena for our decaying system are related mathematically to the initial value problem of the time-dependent Schrödinger equation,

$$i \frac{\partial \psi(\mathbf{r}, t)}{\partial t} + \frac{\nabla^2 \psi(\mathbf{r}, t)}{2} - b\delta(r-a)\psi(\mathbf{r}, t) = 0, \quad (5)$$

with initial wave functions $\psi(\mathbf{r})$ at $t=0$. This problem can in principle be solved by using the stationary states of the Hamiltonian

$$H\psi_k = u_k\psi_k.$$

Then the formal solution to the problem is given by

$$\psi(\mathbf{r}, t) = \int dk \alpha(k) e^{-iu_k t} \psi_k(\mathbf{r}) \quad \text{with } \alpha(k) = \langle \psi_k, \psi(\mathbf{r}, 0) \rangle,$$

where $\psi(\mathbf{r}, 0)$ is the given initial wave function. This problem, however, is very inefficient for numerical computations [12,13]. Hence we now try to solve Eq. (5) directly.

The solution of Eq. (5) may be found for all the space-time coordinates such that $r \in R$ and $t > 0$ in a certain region R and boundary S . For the S states the wave functions are depended on the radial coordinate only. Substituting $\psi(\mathbf{r}, t)/r$ for $\psi(\mathbf{r}, t)$ in Eq. (5) becomes

$$\frac{\partial \psi(r, t)}{\partial t} - \frac{1}{2} \frac{\partial^2 \psi(r, t)}{\partial r^2} = 0, \quad r \neq a, t > 0, \quad (6)$$

with boundary conditions

$$\psi(0, t) = 0 \quad \text{for } t \geq 0,$$

$$\frac{\partial \psi(a+,t)}{\partial r} - \frac{\partial \psi(a-,t)}{\partial r} = 2b\psi(a,t), \quad (7)$$

and the initial condition [11]

$$\begin{aligned} \psi(r,0) &= \alpha_1 [e^{(ik-\mu)r} - e^{-(ik-\mu)r}] \quad \text{for } r \leq a, \\ &= \alpha_2 e^{(ik-\mu)r} \quad \text{for } r \geq a. \end{aligned} \quad (8)$$

The function $\psi(r,t)$ is required to be continuous for $r \in [0, +\infty)$ and $t > 0$. For any positive integer L and M let $\psi_{Lj}(t) = \psi(jh,t), j=0,1,\dots,L,\dots,M$, where the following conditions are required: $Lh=a$. The semidiscretization involves representing $\partial^2 \psi(r,t)/\partial r^2$ at the points (jh,t) in terms of $\psi_j(t), \psi_{j-1}(t)$ and $\psi_{j+1}(t)$. Substituting in Eq. (6) one obtains a system of ordinary differential equations involving the dependent variables $\psi_1(t), \psi_2(t), \dots, \psi_{L-1}(t), \psi_{L+1}(t), \dots, \psi_{M-1}(t)$. Thus, for example, if we let

$$\frac{\partial^2 \psi_j(t)}{\partial t^2} \approx \frac{\psi_{j+1}(t) + \psi_{j-1}(t) - 2\psi_j(t)}{h^2},$$

then we obtain, upon substitution in Eq. (6), the system of ordinary differential equations

$$\frac{d\psi_j(t)}{dt} = -\frac{i}{2} \frac{\psi_{j+1}(t) + \psi_{j-1}(t) - 2\psi_j(t)}{h^2}. \quad (9)$$

From Eqs. (7) and (8) we have

$$\psi_0(t) = 0 \quad (10)$$

and

$$\begin{aligned} \psi_j(0) &= \alpha_1 [e^{(ik-\mu)hj} - e^{-(ik-\mu)hj}] \quad \text{for } j < L, \\ &= \alpha_2 e^{(ik-\mu)hj} \quad \text{for } j > L. \end{aligned} \quad (11)$$

For $j=L$ we obtain the wave function from Eq. (7),

$$\psi_L(t) = \frac{1}{2b} \left[\left. \frac{\partial \psi(r,t)}{\partial r} \right|_{j=L+1} - \left. \frac{\partial \psi(r,t)}{\partial r} \right|_{j=L-1} \right] \quad (12)$$

where

$$\left. \frac{\partial \psi(r,t)}{\partial r} \right|_{j=L+1} = \frac{\psi_{L+2}(t) - \psi_{L+1}(t)}{h} \approx \left. \frac{\partial \psi(r,t)}{\partial r} \right|_{r=a+3h/2}$$

and

$$\left. \frac{\partial \psi(r,t)}{\partial r} \right|_{j=L-1} \approx \frac{\psi_{L-1}(t) - \psi_{L-2}(t)}{h} = \left. \frac{\partial \psi(r,t)}{\partial r} \right|_{r=a-3h/2}.$$

Although we actually need $\partial \psi/\partial r$ at $j=L \pm 1$ in Eq. (12), these differ from the derivatives at $j=L+3/2$ only by 0.01%. This estimate was made by evaluating $\partial^2 \psi/\partial r^2$ in terms of $\partial \psi/\partial r$, using the Schrödinger equation. Equations (9)–(12) are systems of initial value ordinary differential equations. Let us consider the forward difference method

$$\psi_j(t + \Delta t) = \psi_j(t) - \frac{i\Delta t}{2h^2} [\psi_{j+1}(t) + \psi_{j-1}(t) - 2\psi_j(t)].$$

Mesh ratio d is given by

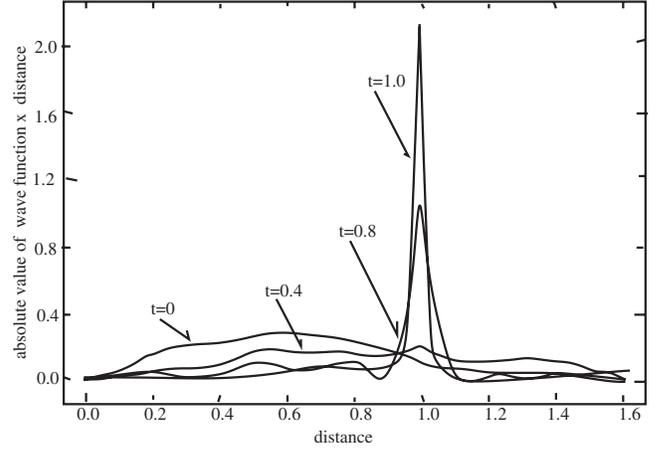


FIG. 1. Time-dependent phenomena for $n=1$ and $b=1$.

$$d = \frac{i\Delta t}{2h^2}.$$

Since $\psi_0(t)$ is given for all t as well as $\psi_1(0), \dots, \psi_M(0)$, and $\psi_L(\Delta t)$ is evaluated from Eq. (12), then $\psi_1(2\Delta t), \psi_2(2\Delta t)$, etc. We used this method with the condition $|d| < 1/2$ for stability.

The numerical values of time-dependent wave functions are evaluated and shown in Figs. 1 and 2 for $b=1$. The peak shown in Fig. 1 appears around $t=1.0$, afterwards the sharp shot decreases and the width widens substantially in a time reverse manner against $t=1.0$ which is shown in Fig. 2. Here we used interactive graphic technology to observe the peak arising during the real time process by utilizing powerful open GL under G++ (object oriented GNU C language) program language environment in open SUSE Linux 10.2 operating system of 64 bit kernel. We retained less than 2% overall accuracy for the evaluation of the wave functions for the lowest S states. Initially we discretized at each 0.1 interval, then we obtained the corresponding second-order difference equations with respect to time variable t . First we let $\Delta t = 0.1$, then we let Δt be a half of the previous Δt . We obtained the deviation of the magnitudes of the wave functions

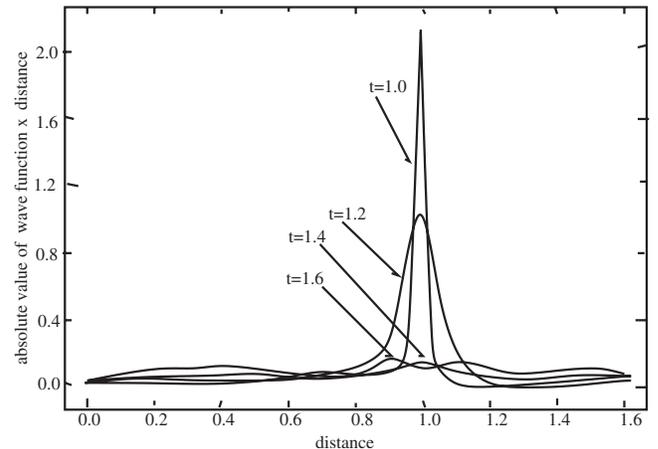


FIG. 2. Time-dependent phenomena for $n=1$ and $b=1$.

using these two different time steps at the same fixed time for all the semidiscretization points of r , then we averaged the relative differences of the absolute values of the wave functions over these semidiscretization points. In case these average relative difference became more than 2% we divided the time steps into another half of the previous time interval Δt , and solved the corresponding time-dependent second-order difference equation. Again the above procedure tested whether the relative accuracy was within 2%. We repeated these processes until the overall accuracy reached within 2% up to 64 times. If after 64 times repetition the overall accuracy did not fall within 2%, we reduced the distance interval, h , to a half of the previous value, then we tried the above-mentioned procedure again up to 64 times.

Finally, in the case for true single particle wave functions of the lowest energy level of S states, the functions would be concave toward the x axis everywhere and would not change curvature from convex toward concave. However, our system is actually an adaptation of interactive more than one particle system by using the hypothetical model potential of a three-dimensional δ shell. Hence as shown in Fig. 1, even at $t=0$, there seems to be a slightly different form of wave shapes.

In conclusion, we solved time-dependent Schrödinger wave equations for the decaying system. We realized that after $t=0.5$ the probability of finding the particle inside the potential is considerably less than that of the corresponding initial decaying state. From then on there is no appreciable change of the probability inside the potential up to the largest time for which the solution was evaluated. This implies that the particle initially inside the potential is leaking out rather rapidly at early times and then less rapidly as time progresses. Hence we calculated relatively small values of time in order to observe the more apparent behavior of the

time-dependent phenomena. The results for the $n=1$ and $b=1$ case are shown in Figs. 1 and 2. At $t=0.2$ the shape of the wave function is similar to the initial state. This implies that before $t=0.2$ there is no significant time-dependent phenomena of the particle. After this time the shape of the wave function becomes more complicated, and a small peak is observed near $r=1$. A possible interpretation of this is that the particle initially inside the potential barrier attempts to tunnel out through the potential shell; however, the barrier is repulsive at this time at this point, preventing the particle from leaking out easily. This causes a time delay effect of the particle inside the barrier, explaining the occurrence of the peak near the repulsive potential barrier. As time progresses the peak near $r=1$ grows higher and also the width decreases correspondingly. Around $t=1$ this peak is highest and steepest. Afterwards the probability of finding the particle inside the potential barrier becomes smaller and the peak also becomes smaller. After $t=1.6$ there is no appreciable peak observable and the magnitude of the wave function inside the potential barrier becomes considerably smaller due to the leak out of the particle through the potential. These observations predict that the decaying behaviors of our model case is similar to those of typical few-body systems.

From the results of these calculations we finally conclude that our nonequilibrium many-body Green function approaches will be applicable to the resonance behaviors of real few particle systems beyond model cases. Compared with other approaches, our methods may not be the simplest and the most efficient way to the decaying problems. However, the merits of our Liouvillian Green techniques are more algebraic in nature and adapted intrinsically far from equilibrium. Hence we expect that our procedure will be applicable in the broader realms of resonance scattering phenomena in a unifying way, at least in the conceptual view points.

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