Nonequlibrium Green-function-based resonance system

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The Tani transformation is used for the representation of the Hamiltonian to a decaying system with bound states. We considered the Liouvillean Green function and self-energy for a system far from equilibrium. Then we express the many-body Green function in terms of expectation values of decaying system operators. Next we considered that the solutions obtained from the variational stabilization process with functional derivative correspond to the resonant poles for the decaying system. This adapted variation of the procedure is applied to our model potential of three-dimensional δ barriers. We evaluated the poles for S states and the corresponding initial-state wave functions for this potential.

I. INTRODUCTION

In decaying processes, there are several different theoretical approaches. However, all of them have in common that the sharp variation of the cross section near the resonant energy is in a certain way related to the existence of quasibound states of the resonant system. When a particle with resonant energy is scattered, it may be in a certain period of time captured into this quasibound state, which causes abrupt variations in the total cross section. In the complex momentum plane the momentum values lie on the positive imaginary axis for the bound states and those lying in the lower half of the complex momentum plane correspond to the asymtotically exponentially diverging functions which are called Gamow-Siegert resonances [1,2]. Since then, complex coordinate techniques (rotation [3–7], stabilization [8–11]) have been widely used to evaluate the resonance parameters. More recently close-coupling methods [12,13] have been used for resonant processes such as atomic collisions, etc. In this paper we applied the Liouvillean Green function method [14] to the noncollective theory of resonant phenomena. This formulation is intrinsically far from equilibrium and has been applied to collective phenomena of the theory of spectral line shapes [15].

II. TANI HAMILTON FORMULATION

There are many systems of composite particles for which composite particle operators are convenient for the representation of the Hamiltonian explicitly in terms of individual particle operators. The Tani transformation [16] is one of the several methods for this purpose. This is the method used in this section, with the notation adapted to our problem.

Let us consider a single-particle resonance scattering system with bound states. Let $\psi_\alpha(\mathbf{r})$ be the initial wave functions of the decaying states. These states can be represented using decaying-state annihilation and creation operators $\hat{F}_\alpha$ and $\hat{F}_\alpha^\dagger$, respectively. The corresponding bound-state operators $\hat{\mu}_\alpha$ and $\hat{\mu}_\alpha^\dagger$, respectively, satisfy Bose commutation relations. A precise definition of these operators can be given by making use of an enlarged state space [16].

We now try to find a unitary transformation $\hat{O}$ which shifts the description of decaying states to the bound-state operators. The reason for this is that the bound-state operators have simple commutation relations with the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$ in contrast with the complex commutation relations between the decaying-state operators and field operators. The creation and annihilation operators for the αth decaying state of a quantum-mechanical one-particle system are

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

where the field operators themselves 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 the 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 $\hat{\mu}_\alpha$,

$$\hat{\mu}_\alpha(\varepsilon) = \hat{O}^{-1}(\varepsilon)\hat{\mu}_\alpha\hat{O}(\varepsilon),$$

then the derivative of the transformed bound operator becomes

$$\frac{d\hat{\mu}_\alpha(\varepsilon)}{d\varepsilon} = -\hat{F}_\alpha(\varepsilon). \tag{1}$$

The commutator of $\hat{F}_\alpha$ and $\hat{B}$ is given by $[\hat{F}_\alpha, \hat{B}] = \hat{\mu}_\alpha$, and the derivative of the transformed decaying-state operator satisfies

$$\frac{d\hat{F}_\alpha(\varepsilon)}{d\varepsilon} = \hat{\mu}_\alpha(\varepsilon). \tag{2}$$

By elimination of the operator $\hat{F}_\alpha$ from Eqs. (1) and (2) and using the initial conditions $\hat{\mu}_\alpha(0) = \hat{\mu}_\alpha$ and $\hat{\mu}'_\alpha(0) = -\hat{F}_\alpha$, we have

$$\hat{\mu}_\alpha(\varepsilon) = \hat{\mu}_\alpha \cos \varepsilon - \hat{F}_\alpha \sin \varepsilon. \qquad (3)$$

From Eq. (3), if we let ε be $\pi/2$, $\hat{\mu}_\alpha(\pi/2) = -\hat{F}_\alpha$. Hence the bound operators can be expressed in terms of the excited-state operators. Let $\hat{O}$ the transformation for $\varepsilon = \pi/2$, $\psi_\mathbf{k}(\mathbf{r})$ the normalized free-particle wave function with wave vector $\mathbf{k}$, and $\hat{\mu}_\mathbf{k}$ and $\hat{\mu}_\mathbf{k}^\dagger$ the free-particle annihilation and creation operators, respectively. Then the transformed field operator gives

$$\hat{O}^{-1}\hat{\psi}\hat{O} = \sum_\alpha \psi_\alpha(\mathbf{r})\hat{\mu}_\alpha - \int d\mathbf{k} \int d\mathbf{r}' \Delta(\mathbf{r},\mathbf{r}')\psi_\mathbf{k}(\mathbf{r}')\hat{\mu}_\mathbf{k}$$
$$+ \int d\mathbf{k}\, \psi_\mathbf{k}(\mathbf{r})\hat{\mu}_\mathbf{k}, \qquad (4)$$

where $\Delta(\mathbf{r}_1,\mathbf{r}_2) = \Sigma_\alpha \psi_\alpha(\mathbf{r}_1)\psi_\alpha^*(\mathbf{r}_2)$. We now obtain the Tani Hamiltonian by using the transformed field operators:

$$\hat{H}_{(\text{Tani})} = \int d\mathbf{r}[\hat{O}^{-1}\hat{\psi}(\mathbf{r})\hat{O}]^\dagger H(\mathbf{r})[\hat{O}^{-1}\hat{\psi}(\mathbf{r})\hat{O}].$$

By using Eq. (4), after some arrangement we finally have the Tani Hamiltonian which takes the bound states explicitly into consideration:

$$\hat{H}_{(\text{Tani})} = \sum_{\alpha,\beta} \int d\mathbf{r}\,\psi_\alpha^*(\mathbf{r})H(\mathbf{r})\psi_\beta(\mathbf{r})\hat{\mu}_\alpha^\dagger\hat{\mu}_\beta + \int d\mathbf{k} \int d\mathbf{k}' \int d\mathbf{r}' \int d\mathbf{r}'' \int d\mathbf{r}\,\Delta(\mathbf{r}',r)H(\mathbf{r})\Delta(\mathbf{r},r'')\psi_\mathbf{k}^*(\mathbf{r}')\psi_{\mathbf{k}'}(\mathbf{r}'')\hat{\mu}_\mathbf{k}^\dagger\hat{\mu}_{\mathbf{k}'}$$
$$+ \int d\mathbf{k} \int d\mathbf{k}' \int d\mathbf{r}\,\psi_\mathbf{k}^*(\mathbf{r})H(\mathbf{r})\psi_{\mathbf{k}'}(\mathbf{r})\hat{\mu}_\mathbf{k}^\dagger\hat{\mu}_{\mathbf{k}'} - \sum_\alpha \int d\mathbf{k} \int d\mathbf{r}' \int d\mathbf{r}\,\psi_\alpha^*(\mathbf{r})H(\mathbf{r})\Delta(\mathbf{r},r')\psi_\mathbf{k}(\mathbf{r}')\hat{\mu}_\alpha^\dagger\hat{\mu}_\mathbf{k}$$
$$- \sum_\alpha \int d\mathbf{k} \int d\mathbf{r}' \int d\mathbf{r}\,\Delta(\mathbf{r}',r)H(\mathbf{r})\psi_\alpha(\mathbf{r})\psi_\mathbf{k}^*(\mathbf{r}')\hat{\mu}_\mathbf{k}^\dagger\hat{\mu}_\alpha + \sum_\alpha \int d\mathbf{k} \int d\mathbf{r}\,\psi_\alpha^*(\mathbf{r})H(\mathbf{r})\psi_\mathbf{k}(\mathbf{r})\hat{\mu}_\alpha^\dagger\hat{\mu}_\mathbf{k}$$
$$+ \sum_\alpha \int d\mathbf{k} \int d\mathbf{r}\,\psi_\mathbf{k}^*(\mathbf{r})H(\mathbf{r})\psi_\alpha(\mathbf{r})\hat{\mu}_\mathbf{k}^\dagger\hat{\mu}_\alpha - \int d\mathbf{k} \int d\mathbf{k}' \int d\mathbf{r}' \int d\mathbf{r}\,\Delta(\mathbf{r}',r)H(\mathbf{r})\psi_{\mathbf{k}'}(\mathbf{r})\psi_\mathbf{k}^*(\mathbf{r}')\hat{\mu}_\mathbf{k}^\dagger\hat{\mu}_{\mathbf{k}'}$$
$$- \int d\mathbf{k} \int d\mathbf{k}' \int d\mathbf{r}' \int d\mathbf{r}\,\psi_\mathbf{k}^*(\mathbf{r})H(\mathbf{r})\Delta(\mathbf{r},r')\psi_{\mathbf{k}'}(\mathbf{r}')\hat{\mu}_\mathbf{k}^\dagger\hat{\mu}_{\mathbf{k}'}. \qquad (5)$$

III. SELF-ENERGY

In the previous section we adapted Tani's derivation of a single-particle canonically transformed Hamiltonian to our case of a decaying system with bound states. We now briefly review the Green function and self-energy for a system far from equilibrium. The usual quantum field theory developed for application to the many-body problem [17,18] is based on thermodynamic equilibrium, which is not well adapted to nonequilibrium phenomena. The Liouvillean Green functions, which we are going to describe here, are based on the transition-state operators, which are especially suitable for nonequilibrium systems such as dense plasma, intense laser beams, and decaying states. This nonequilibrium Green function technique has been applied to the theory of spectral line shapes [15]; however, because of a lack of translational symmetry, applications of this method to the theory of decaying systems are more complex.

Using the Liouvillean operator $\hat{L}$, the Heisenberg equation of motion for $\hat{F}_\alpha$ is given as

$$i\frac{\partial \hat{F}_\alpha(t)}{\partial t} = [\hat{F}_\alpha(t),\hat{H}] = \hat{L}\hat{F}_\alpha(t). \qquad (6)$$

The Liouvillean Green function is expressed in terms of expectation values of the 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 Liouvillean 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:

$$\hat{L}\hat{F}_\alpha = [\hat{F}_\alpha,\hat{H}] = \sum_\alpha \gamma(\alpha|n)\hat{\tau}_n. \qquad (7)$$

From Eqs. (6) and (7) and using the Laplace transformation, we obtain the transformed Green functions

$$z\tilde{G}(\alpha,z|\alpha,0) - \sum_n \gamma(\alpha|n)\tilde{G}(n,z|\alpha,0) = iG(\alpha,0|\alpha,0),$$

$$z\widetilde{G}(n,z|\alpha,0) - \sum_{n'} \gamma(n|n')\widetilde{G}(n',z|\alpha,0) = iG(n,0|\alpha,0). \quad (8)$$

In the case of no decaying states, from Eq. (8), all the off-diagonal elements of the Liouvillean functions with respect to the basis, $\gamma(\alpha|n)$ and $\gamma(n|n')$ ($n \neq n'$), vanish and we obtain the free Green functions

$$\widetilde{G}_0(\alpha,z|\alpha,0) = (z - u_\alpha)^{-1}iG(\alpha,0|\alpha,0),$$

$$\widetilde{G}_0(n,z|\alpha,0) = (z - u_n)^{-1}iG(n,0|\alpha,0). \quad (9)$$

Let us assume that $G(\alpha,t|\alpha,0)$ increases less rapidly than exponentially as t approaches $+\infty$; then, the Laplace transforms of $\widetilde{G}(\alpha,z|\alpha,0)$ will be analytic in the upper-half complex energy plane. For a decaying system the analytical continuation of $\widetilde{G}(\alpha,z|\alpha,0)$ 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 $\widetilde{G}(\alpha,z|\alpha,0)$ we can propose the following form of the Green functions:

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

where $\Sigma_\alpha(z)$ will be called the self-energy. By iteration [14] of Eq. (9) the perturbation expansion of $\widetilde{G}(\alpha,z|\alpha,0)$ is

$$\widetilde{G}^{(l)}(\alpha,z|\alpha,0) = \frac{i}{z_\alpha - u_\alpha}$$
$$\times \sum_{n_1,\ldots,n_l}{}' \frac{\gamma(\alpha|n_1)\cdots\gamma(n_{l-1}|n_l)G(n_l,0|\alpha,0)}{(z - u_{n_1})\cdots(z - u_{n_l})}. \quad (10)$$

This implies a perturbation expansion of Σ_α, which is, up to second order, $\Sigma_\alpha = \Sigma_\alpha^{(1)} + \Sigma_\alpha^{(2)} + \cdots$, with

$$\Sigma_\alpha^{(1)}(z) = \frac{(z - u_\alpha)^2 \widetilde{G}^{(1)}(\alpha,z|\alpha,0)}{iG(\alpha,0|\alpha,0)},$$

$$\Sigma_\alpha^{(2)}(z) = \frac{(z - u_\alpha)^2 \widetilde{G}^{(2)}(\alpha,z|\alpha,0)}{iG(\alpha,0|\alpha,0)} - \frac{[\Sigma_\alpha^{(1)}(z)]^2}{z - u_\alpha}. \quad (11)$$

There may exist an infinite set of operator bases which are degenerate with the operators $\hat{F}_\alpha$ in the unperturbed approximation, so it is important to separate these resonance contributions from the nonresonance [14] ones. Then using Eq. (10) the first-order expression [14] in Eqs. (11) becomes

$$\sum_{\alpha}^{(1)}(z) = \sum_{n \in \text{res}}{}' \gamma(\alpha|n)\frac{G(n,0|\alpha,0)}{G(\alpha,0|\alpha,0)} + (z - u_\alpha)$$
$$\times \sum_{n \notin \text{res}} \frac{\gamma(\alpha|n)G(n,0|\alpha,0)}{(z - u_n)G(\alpha,0|\alpha,0)}, \quad (12)$$

where "res" denotes the resonance contributions. Near the resonance poles the resonance terms contribute to the resonance poles only through the second order. Hence using Eqs. (10) and (11) we obtain the second-order contribution:

$$\sum_{\alpha}^{(1)}(z) = (z - u_\alpha)\sum_{n,n'}{}' \frac{\gamma(\alpha|n)\gamma(n|n')G(n,0|\alpha,0)}{(z - u_n)(z - u_{n'})G(\alpha,0|\alpha,0)}$$
$$-\frac{\left[\sum_{\alpha}^{(1)}(z)\right]^2}{z - u_\alpha}.$$

By separating the resonant and nonresonant contributions, substituting Eq. (12) for $\Sigma_\alpha^{(1)}$, and after rearrangement, we derive the self-energy through the second order [14],

$$\sum_{\alpha}^{(2)}(z) = \int d\mathbf{k} \frac{\gamma(\alpha|\mathbf{k})\gamma(\mathbf{k}|n)}{u_\alpha - \frac{1}{2}k^2 + i\iota}, \quad (13)$$

where we used free-particle creation and annihilation operators as the basis operators, and for decaying systems the first-order self-energy vanishes. From the Tani Hamiltonian, Eqs. (5) and (7), we can evaluate the matrix elements of the Liouvillean operator. Then,

$$\gamma(\alpha|\mathbf{k})\gamma(\mathbf{k}|\alpha) = \sum_{\beta\beta'} \int d\mathbf{r} \int d\mathbf{r}' \psi_\beta^*(\mathbf{r})[\delta_{\alpha\beta}H(\mathbf{r}) - u_{\alpha\beta'}]$$
$$\times \psi_\mathbf{k}(\mathbf{r})\psi_\mathbf{k}^*(\mathbf{r}')[\delta_{\alpha\beta'}H(\mathbf{r}') - u_{\beta'\alpha}]\psi_{\beta'}(\mathbf{r}'). \quad (14)$$

Here we are concerned about the decaying states, and in the first approximation we can regard the individual decaying states as independent of each other; hence, the off-diagonal elements of Eq. (14) are neglected. Then,

$$\gamma(\alpha\mathbf{k})\gamma(\mathbf{k}\alpha) = \int d\mathbf{r} \int d\mathbf{r}' \psi_\alpha^*(\mathbf{r})[H(\mathbf{r}) - u_\alpha]$$
$$\times \psi_\mathbf{k}(\mathbf{r})\psi_\mathbf{k}^*(\mathbf{r}')[H(\mathbf{r}') - u_\alpha]\psi_\alpha(\mathbf{r}'). \quad (15)$$

Substituting Eq. (15) into Eq. (13), one finds

$$\sum_{\alpha}^{(2)}(z) = -\int d\mathbf{r}\psi_\alpha^*(\mathbf{r})[H(\mathbf{r}) - u_\alpha]\psi_\alpha(\mathbf{r})$$
$$-\int d\mathbf{r}\psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})\psi_\alpha(\mathbf{r})$$
$$+\int d\mathbf{r} \int d\mathbf{r}' \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})G_\alpha(\mathbf{r},r')\zeta(\mathbf{r}')\psi_\alpha(\mathbf{r}'), \quad (16)$$

where

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

IV. FUNCTIONAL VARIATION

When the variational technique is applied to a real functional, the method is related to the extremum of the functional with respect to the variation of function. If the functional is a complex-valued function, there exists neither an upper nor a lower bound [10,19]. Let us consider trial wave functions [20]. The variation process is related to the least variation of trial functions. If we extend this stabilization process to the exact variational method with a functional derivative, we suggest that the solutions obtained from this variational process correspond 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. In this respect our decaying-state wave functions are different from Gamow-Siegert states which are non-normalizable outgoing waves. Using Eq. (16),

$$z_\alpha - \lambda_\alpha(\psi_\alpha, \psi_\alpha) = \int d\mathbf{r}\, \psi_\alpha^*(\mathbf{r})H(\mathbf{r})\psi_\alpha(\mathbf{r}) - \int d\mathbf{r}\, \psi_\alpha^*(\mathbf{r})[H(\mathbf{r})$$

$$- u_\alpha]\psi_\alpha(\mathbf{r}) - \int d\mathbf{r}\, \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})\psi_\alpha(\mathbf{r})$$

$$+ \int d\mathbf{r} \int d\mathbf{r}'\, \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})G_\alpha(\mathbf{r},\mathbf{r}')$$

$$\times \zeta(\mathbf{r}')\psi_\alpha(\mathbf{r}') - \lambda_\alpha(\psi_\alpha, \psi_\alpha). \quad (17)$$

Now we define the functional derivative

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

where $\delta F[\psi] = F[\psi(\chi) + \lambda\delta(\chi - \chi')] - F[\psi]$. Using Eq. (17),

$$\frac{\delta \int d\mathbf{r}\, \psi_\alpha^*(\mathbf{r})H(\mathbf{r})\psi_\alpha(\mathbf{r})}{\delta\psi_\alpha^*(\mathbf{r})}$$

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

$$+ H(\mathbf{r})\psi_\alpha(\mathbf{r}) \int d\mathbf{r} \int d\mathbf{r}'\, \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})\frac{\partial G_\alpha(\mathbf{r},\mathbf{r}')}{\partial u_\alpha}$$

$$\times \zeta(\mathbf{r}')\psi_\alpha(\mathbf{r}')\frac{\delta\lambda_\alpha \int d\mathbf{r}\, \psi_\alpha^*(\mathbf{r})\psi_\alpha(\mathbf{r})}{\delta\psi_\alpha^*(\mathbf{r})}$$

$$= \lambda_\alpha \psi_\alpha(\mathbf{r}).$$

Hence the variational equation $\delta[z_\alpha - \lambda_\alpha(\psi_\alpha, \psi_\alpha)] = 0$ leads to

$$-\frac{1}{2}\left[1 + \int d\mathbf{r} \int d\mathbf{r}'\, \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})\frac{\partial G_\alpha(\mathbf{r},\mathbf{r}')}{\partial u_\alpha}\zeta(\mathbf{r}')\psi_\alpha(\mathbf{r}')\right]$$

$$\times \nabla^2\psi_\alpha(\mathbf{r}) + \zeta(\mathbf{r})$$

$$\times \left[\int d\mathbf{r} \int d\mathbf{r}'\, \psi_\alpha^*(\mathbf{r})\zeta(\mathbf{r})\frac{\partial G_\alpha(\mathbf{r},\mathbf{r}')}{\partial u_\alpha}\zeta(\mathbf{r}')\psi_\alpha(\mathbf{r}')\right]\psi_\alpha(\mathbf{r})$$

$$+ \zeta(\mathbf{r})\int d\mathbf{r}'\, G_\alpha(\mathbf{r},\mathbf{r}')\zeta(\mathbf{r}')\psi_\alpha(\mathbf{r}') = (\lambda_\alpha - u_\alpha)\psi_\alpha(\mathbf{r}), \quad (18)$$

where we used atomic units $m = \hbar = e = 1$. Let

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

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

Then Eq. (18) can be finally written as

$$-\frac{(1+\kappa)}{2}\nabla^2\psi_\alpha(\mathbf{r}) + \zeta(\mathbf{r})\kappa\psi_\alpha(\mathbf{r}) + \zeta(\mathbf{r})\xi(\mathbf{r}) = (\lambda_\alpha - u_\alpha)\psi_\alpha(\mathbf{r}). \quad (19)$$

At this point, if we disregard the nonlinear factors with respect to $\psi_\alpha(\mathbf{r})$ and $\psi_\alpha^*(\mathbf{r})$ and let the coefficients κ and $\xi(\mathbf{r})$ be constant with respect to these wave functions, the nonlinear decaying-state wave equation (18) is reduced into the corresponding nondecaying Schrödinger wave equation. Hence nonlinearity plays a crucial role in our decaying system.

V. APPLICATION OF THE VARIATIONAL TECHNIQUE TO THE THREE-DIMENSIONAL δ POTENTIAL

We now apply the variational method described in the last section to our model potential: the three-dimensional δ barrier. This potential can roughly be regarded as a model potential for a particle tunneling out of a metastable excited resonance atom. Let us consider a single spinless boson particle tunneling out of the potential, $b\delta(r-a)$, where a, b are positive real numbers. The scattering problem which is related to this potential can also be found in Gottfried's book [21].

Let us consider the S-state wave functions $\psi_\alpha(r)$. For an S state the wave equation using spherical coordinates, Eq. (19), becomes

$$-\frac{(1+\kappa)}{2}\nabla^2\psi_\alpha(r) + [b\kappa\psi_\alpha(a) + \xi]\delta(r-a) = (\lambda_\alpha - u_\alpha)\psi_\alpha(r), \quad (20)$$

where κ and $\xi(r)$ are evaluated as

$$\kappa = \frac{i4\pi b^2 a^2|\psi_\alpha(a)|^2}{(\sqrt{2u_\alpha})^3}[e^{i2a\sqrt{2u_\alpha}}i(2a\sqrt{2u_\alpha}-1)+1], \quad (21)$$

$$\xi(r) = -ba^2\psi_\alpha(a)\int_0^\pi d\theta \frac{\sin\theta e^{i\sqrt{2u_\alpha}\sqrt{r^2-2\arccos\theta+a^2}}}{\sqrt{r^2-2\arccos\theta+a^2}}.$$

By using the identity $\delta(r-a)\psi(r)=\delta(r-a)\psi(a)$,

$$\zeta(r)\xi(r) = -b^2a^2\psi_\alpha(a)\int_0^\pi d\theta \frac{\sin\theta e^{i\sqrt{2u_\alpha}\sqrt{2a^2(1-\cos\theta)}}}{\sqrt{2a^2(1-\cos\theta)}}\delta(r-a).$$

By substitution of μ for $\cos\theta$ and t for $\sqrt{1-\mu}$, the integral can be evaluated easily, and one finds finally

$$\zeta(r)\xi(\mathbf{r}) = \frac{ib^2\psi_\alpha(a)}{\sqrt{2u_\alpha}}[e^{i2a\sqrt{2u_\alpha}}-1]\delta(r-a).$$

If we let $\zeta(r)\xi(\mathbf{r})=d\delta(r-a)$, then

$$\xi = \frac{ib^2\psi_\alpha(a)}{\sqrt{2u_\alpha}}[e^{i2a\sqrt{2u_\alpha}}-1]. \quad (22)$$

The solution of Eq. (20) is continuous at $r=a$; however, the slope of the solution is not continuous and forms a cusp at the same point due to the contribution of the δ function. Let $\widetilde{\psi}(r)=\psi(r)/r$. Integrating the equation from $a-\varepsilon$ to $a+\varepsilon$ for a small positive ε and letting $\varepsilon=0$, one finds

$$-\frac{(1+\kappa)}{2}[\widetilde{\psi}'(a+)-\widetilde{\psi}'(a-)]+b\kappa\widetilde{\psi}(a)+a\xi=0, \quad (23)$$

denoting $\widetilde{\psi}'(a+)$ and $\widetilde{\psi}'(a-)$ by the right and left-hand derivatives with respect to r at $r=a$, respectively.

Generally we cannot solve the nonlinear wave equation in closed form and must resort to numerical computation. However, in the case of the present potential, the exact analytical form can be determined as follows. For the resonant wave functions corresponding to the S states ($l=0$), there exists an exact form of the normalizable solution of the wave equation for $r\neq a$. However, the δ potential term in Eq. (20) contributes to the discontinuity of the slope of the wave function; hence, we obtain Eq. (23). We can satisfy this equation by using the attenuation parameter μ,

$$r\leqslant a, \psi(r) = \alpha_1\frac{e^{(ik-\mu)r}-e^{-(ik-\mu)r}}{r},$$

$$r\geqslant a, \psi(r) = \alpha_2\frac{e^{(ik-\mu)r}}{r}, \quad (24)$$

where α_1 and α_2 are complex coefficients to be determined by the requirement of continuity at $r=a$ and normalization of wave functions through the three-dimensional space. Let us consider the continuity requirement at $r=a$,

By transposition and normalization requirements, one obtains finally

$$\alpha_1^2 = \frac{1}{4\pi[e^{2\mu a}-\cos(2ak)/\mu-\sin(2ak)/k]}, \quad (25)$$

where α_1 is chosen to be a positive real number.

By substituting Eqs. (21), (22), and (25) into Eq. (23) the wave equation (23) is reduced to two simultaneous algebraic equations with the unknown parameters μ and k.

Next we evaluate the energy

$$u = \int_0^\infty dr 4\pi r^2\psi^*(r)H(r)\psi(r).$$

By expressing the Laplacian with spherical coordinates and using the Hermitian property of $(1/i)(d/dr)$,

$$u = \pi\alpha_1^2(\mu^2+k^2)\left[\frac{e^{2\mu a}-e^{-2\mu a}}{\mu}+\frac{2\sin(2ak)}{k}\right]$$
$$+\pi|\alpha_2|^2 e^{-2\mu a}\left[\frac{\mu^2+k^2}{\mu}+4b\right].$$

Before solving this let us describe the bound states of the system with an infinite wall at $r=a$. The Schrödinger wave equation for the bound states is

$$-\frac{1}{2r}\frac{d^2}{dr^2}r\widetilde{\psi}(r) = u\widetilde{\psi}. \quad (26)$$

The wave function

$$\widetilde{\psi}(r) = \frac{\alpha_1\sin(\sqrt{2ur})+\alpha_2\cos(\sqrt{2ur})}{r}$$

satisfies Eq. (26). It is required that the wave functions remain finite as r approaches zero and that $\widetilde{\psi}(a)=0$. This leads, along with normalization, to

$$\widetilde{\psi}(r) = \frac{1}{\sqrt{2\pi}}\frac{\sin(n\pi r/a)}{r},$$

where

$$n = 1,2\ldots, \quad u_n = \frac{n^2\pi^2}{2a^2}.$$

By letting b approach $+\infty$ we see that the δ barrier problem is reduced to the above-mentioned bound-state problem,

$$\text{potential energy} = \int_0^\infty dr\widetilde{\psi}^*(r)b\delta(r-a)\widetilde{\psi}(r)4\pi r^2$$

$$= 4\pi a^2|\widetilde{\psi}(a)|^2 b.$$

In order that the potential energy remain finite for $b=+\infty$, the wave function at $r=a$ should vanish; hence, the decaying system becomes the corresponding bound-state problem.

We solved the algebraic equation (23) by an iterative procedure in the Linux system. The accuracy of the values μ and k affected significantly the overall accuracy of the wave function, especially as b becomes large. The zero criteria for the algebraic equation (23) should be at least 10^{-6} in order to retain reasonable accuracy of the μ and k values; however, we could not avoid underflow. This problem was solved by using double precision (15 significant digits for the GNU c++ complier). Numerical differentiation can be used for b less than 10, if we guess the initial values of μ and k appropriately; however, if b increases substantially, overflow occurred. With symbolic differentiation we could evaluate b up to 1000 with an accuracy 10^{-10} or better without overflow.
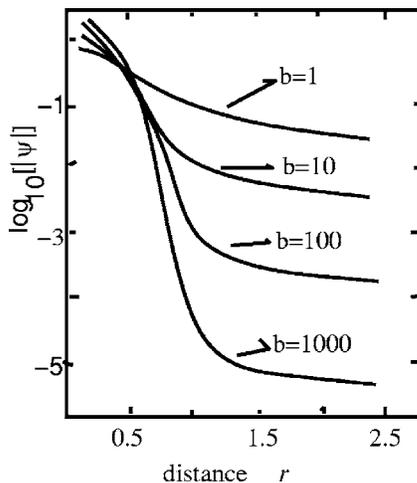
FIG. 1. Initial-state decaying wave ($n=1$).

FIG. 2. Current density ($n=1$ and $b=1$).

For $b=1$ (in units of $\pi^2/2$) the difference between the decaying wave function and the corresponding bound state for the lowest resonance was above 40%. When $b=10$ the difference narrowed down to about 10%. At $b=1000$ the decaying states agreed with the bound states within 0.1%. We evaluated the S states for $n=1$ and $n=2$.

Substituting Eq. (24) into Eq. (17) one obtains the formula for the resonance pole,

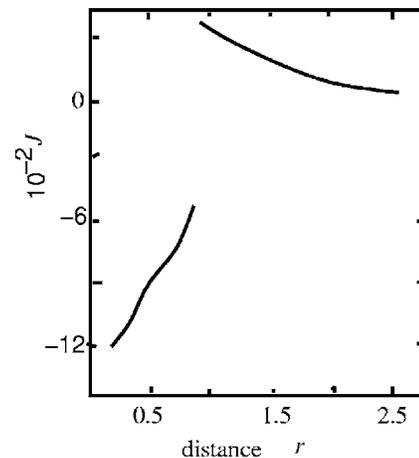$$z = -4\pi|\alpha_2|^2 e^{-2a\mu}b + 4\pi a\alpha_2^* e^{-(ik+\mu)a}\xi = u + \Delta - i\eta.$$

The convergence of the wave functions as b increases is shown in Fig. 1 for $n=1$. The behavior of the current density functions, which are defined by

$$J(r) = \frac{1}{2i}\left[\widetilde{\psi}_{(r)}^* \frac{d\widetilde{\psi}(r)}{dr} - \widetilde{\psi}(r)\frac{d\widetilde{\psi}(r)_{(r)}^*}{dr}\right],$$

is shown in Fig. 2 for $n=1$. We used units with $a=1$ for both figures.

VI. CONCLUSION

In the preceding sections we have presented the formulation of the Liouvillian Green function and self-energy through the second-order perturbation. Using the variational derivative we derived the wave equation for a decaying system. This variational technique was applied to a three-dimensional one-point barrier which is a rough model potential for a particle tunneling out from a metastable atomic system. We evaluated the resonance poles for S states and the corresponding initial-state wave functions for this potential. The solutions found demonstrate especially that our nonlinear wave equation does possess normalizable Gamow-Siegert states, which have physical behavior for r approaching infinity. For the lowest two S states we examined the differences between the transition energy positions for the initial decaying states and the corresponding bound-state energies for various values, and we found that the transition energy position approaches the corresponding bound-state energy as b becomes large. We also examined the global behavior of the wave functions for these two lowest S states. At $b=1$ the integral of the initial-state probability density inside the potential gives a little more than a half of the total probability. As b increases the initial-state decaying wave functions approached the corresponding bound-state wave functions as is the case of the transition energy positions. Figure 2 indicates that at $t=0$ the current inside the potential flows inward and outside the potential it flows outward. One consequence is that shortly before $t=0$ the wave packet inside the barrier is found to be decaying at large times; this means that a "turnaround" occurs at some intermediate time. The wave packet we found at $t=0$ can be thought of as a "snapshot" of a time-dependent wave packet which collapses from infinity at large $t<0$, becoming concentrated inside the barrier. It then proceeds to decay by leaking back out. The behavior of the current versus radius which we found at $t=0$ suggests that the snapshot was taken shortly before the turnaround. Future investigations of solutions of this nonlinear wave equation should study this turnaround phenomena in more detail. A turnaround is expected on the basis of time-reversal arguments; however, the details need to be understood better.

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