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New Variational Principle for Decaying States

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The Hamiltonian of a system containing decaying states is subjected to a nonunitary similarity transformation which introduces the wave functions of these decaying states as well as those of the "antidecaying" dual states explicitly into the representation. The dependence of the Green's-function pole on these wave functions is used to formulate a variational principle for their determination, yielding a non-Hermitian, nonlinear wave equation including self-energy contributions. Explicit solutions are given in a simple example.

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Since, in the usual description with a self-adjoint Hamiltonian, decaying states cannot be eigenstates of the Schrödinger equation, many approaches have been developed which modify this self-adjoint condition. Important examples are (1) use of non-Hermitian boundary conditions as in the theory of Gamow-Siegert states[1,2] and the Kapur-Peierls method[3]; (2) analytical continuation as in the complex rotation or complex stabilization method[4-7]; (3) use of non-Hermitian "effective Hamiltonians" as in the optical potential and related methods; and (4) more unconventional approaches which modify the basic description of quantum mechanics, such as the rigged Hilbert-space formulation.[8] Variational methods have been shown to be useful in conjunction with several of these approaches.[9-11]

In this Letter we report a new procedure, using a particular similarity transformation to give a non-self-adjoint Hamiltonian, for formulating a variational principle which gives a nonlinear, non-Hermitian, Schrödinger-like equation for calculating wave packets describing initial states of decaying particles.[12] This variational principle[13] uses the duality relationship between a decaying state and its time-reversed partner in the choice of similarity transformation. This allows us to clarify the connection with other approaches and better understand the time-reversal duality. Our variational principle is an improvement upon previous ones in that self-energy and environmental effects are included.

The decay of a state $|\varphi_\alpha(t)\rangle$ is characterized by its persistence amplitude

$$g_\alpha(t) = -i\langle\varphi_\alpha(0)|\varphi_\alpha(t)\rangle \tag{1}$$

or by its Laplace transform to the complex energy plane,

$$\tilde{g}_\alpha(z) = \int_0^\infty dt\, g_\alpha(t)e^{izt}. \tag{2}$$

Although adequate for single-particle potential resonances, this definition requires generalization in the case of single or composite particles coupled to a many-particle environment. The most convenient representation for such problems is Fock space. For one composite with n constituents decaying into vacuum, the inner product in (1) is a vacuum expectation value $\langle 0|\hat{A}_\alpha(t)$

$\times \hat{A}_\alpha{}^\dagger|0\rangle$ in which

$$\hat{A}_\alpha{}^\dagger = \int dx_1 \cdots dx_n \varphi_\alpha(x_1 \cdots x_n) \hat{\psi}^\dagger(x_1) \cdots \hat{\psi}^\dagger(x_n), \quad (3)$$

with $\hat{\psi}^\dagger(x_j)$ the field operator creating the jth constituent at position x_j, $\hat{A}_\alpha(t)$ the Heisenberg operator $e^{i\hat{H}t}\hat{A}_\alpha e^{-i\hat{H}t}$, and $\hat{A}_\alpha{}^\dagger = \hat{A}_\alpha{}^\dagger(0)$.

The generalized Tani transformation[14] is a unitary transformation $\hat{U}$ transforming the composite-particle state $\hat{A}_\alpha{}^\dagger|0\rangle$ into an elementary-particle state $\hat{a}_\alpha{}^\dagger|0\rangle$. Decay processes are exhibited as *explicit* interaction terms in the Fock-Tani Hamiltonian $\hat{H} = \hat{U}^{-1}\hat{H}_{\rm Fock}\hat{U}$. For our present purposes it is necessary to generalize $\hat{U}$ to a *nonunitary* similarity transformation $\hat{S}$.[15] We take the Fock-Tani Hamiltonian to be $\hat{S}^{-1}\hat{H}_{\rm Fock}\hat{S}$ with[14]

$$\hat{S} = \exp[(\pi/2)\hat{F}], \quad \hat{F} = \sum_\alpha(\hat{A}_\alpha{}^\dagger \hat{a}_\alpha - \hat{a}_\alpha{}^\dagger \hat{B}_\alpha). \quad (4)$$

In general the φ_α occurring in the $\hat{A}_\alpha{}^\dagger$ include both bound states and resonances, although we shall concentrate on the latter. The $\hat{B}_\alpha$ annihilate composites in the dual states $\overline{\varphi}_\alpha$:

$$\hat{B}_\alpha = \int dX \overline{\varphi}_\alpha(X) \hat{\psi}(x_n) \cdots \hat{\psi}(x_1), \quad (5)$$

where $X = (x_1, \ldots, x_n)$ and the $\overline{\varphi}_\alpha$ are biorthogonal[7] to the φ_α:

$$\int \overline{\varphi}_\alpha(X) \varphi_\beta(X) dX = \delta_{\alpha\beta}. \quad (6)$$

It is not difficult to show that[14, 16]

$$\hat{S}^{-1}\hat{A}_\alpha{}^\dagger|0\rangle = \hat{a}_\alpha{}^\dagger|0\rangle, \quad \langle 0|\hat{B}_\alpha \hat{S} = \langle 0|\hat{a}_\alpha. \quad (7)$$

Although $\hat{H}$ is now non-Hermitian, it has the same real eigenvalues as $\hat{H}_{\rm Fock}$.

Our generalization of (1) to Fock-Tani representation is

$$g_\alpha(t) = -i\langle \hat{a}_\alpha(t)\hat{a}_\alpha{}^\dagger\rangle, \quad (8)$$

where $\hat{a}_\alpha(t)$ is propagated with the Fock-Tani Hamiltonian. Environmental effects can be included by taking $\langle\hat{O}\rangle = {\rm Tr}(\hat{\rho}\hat{O})$. A Liouville-space representation[17] of (8) and (2) is useful. In the case of a state decaying into a continuum, $\tilde{g}_\alpha(z)$ has a branch cut along the real axis and its analytic continuation into the lower half plane has a pole z_α characterizing the decay, whose position is a functional of φ_α and $\overline{\varphi}_\alpha$. This is the basis of our variational method. We require that z_α be stationary under functional variation of $\overline{\varphi}_\alpha$ and φ_α subject to biorthonormality:

$$[\delta/\delta\overline{\varphi}_\alpha(X)][z_\alpha - \sum_{\beta\gamma}\lambda_{\beta\gamma}{}^\alpha \int \overline{\varphi}_\beta(X')\varphi_\gamma(X')dX'] = 0,$$
$$[\delta/\delta\varphi_\alpha(X)][z_\alpha - \sum_{\beta\gamma}\lambda_{\beta\gamma}{}^\alpha \int \overline{\varphi}_\beta(X')\varphi_\gamma(X')dX'] = 0. \quad (9)$$

To obtain more explicit equations one can introduce the self-energy representation

$$\tilde{g}_\alpha(z) = \frac{\langle \hat{a}_\alpha \hat{a}_\alpha{}^\dagger\rangle}{z - \epsilon_\alpha - \Sigma_\alpha(z, \overline{\varphi}_\beta, \varphi_\gamma)}. \quad (10)$$

Here ϵ_α is the "unperturbed" energy $\int\overline{\varphi}_\alpha(X)H(X)\varphi_\alpha(X)dX$ (in general complex), $H(X)$ is the Schrödinger Hamiltonian of the n constituents of φ_α *including their interactions*, and Σ_α is the proper self-energy, which can be conveniently evaluated in Liouville-space representation.[17] z_α is a solution of

$$z_\alpha - \epsilon_\alpha - \Sigma_\alpha(z_\alpha, \overline{\varphi}_\beta, \varphi_\gamma) = 0. \quad (11)$$

Substitution of the functional derivative of (11) into (9) yields

$$(1 - \partial\Sigma_\alpha/\partial z_\alpha)^{-1}[H(X)\varphi_\alpha(X) + \partial\Sigma_\alpha/\partial\overline{\varphi}_\alpha(X)] = \sum_\beta \lambda_{\alpha\beta}{}^\alpha \varphi_\beta(X),$$
$$(1 - \partial\Sigma_\alpha/\partial z_\alpha)^{-1}[\overline{H}(X)\overline{\varphi}_\alpha(X) + \partial\Sigma_\alpha/\partial\varphi_\alpha(X)] = \sum_\beta \lambda_{\beta\alpha}{}^\alpha \overline{\varphi}_\beta(X). \quad (12)$$

Here $\partial\Sigma_\alpha/\partial\overline{\varphi}_\alpha(X)$ is the partial functional derivative of $\Sigma_\alpha(z_\alpha, \overline{\varphi}_\beta, \varphi_\gamma)$ with respect to $\overline{\varphi}_\alpha$ holding z_α, the $\overline{\varphi}_\beta$ with $\beta \neq \alpha$, and all φ_β constant, and similarly for $\partial\Sigma_\alpha/\partial\varphi_\alpha(X)$; $\partial\Sigma_\alpha/\partial z_\alpha$ is the usual partial derivative with respect to z_α. $\overline{H}$ denotes the adjoint with respect to the biorthogonal inner product:

$$\int \overline{f}(X)H(X)g(X)dX = \int g(X)\overline{H}(X)\overline{f}(X)dX. \quad (13)$$

If $H(X)$ is the sum of nonrelativistic kinetic energy and a local potential (no magnetic field or spin) then $\overline{H} = H$. More generally, if we write $H = H(X, P)$ to indicate the dependence on momenta $p_j = i\partial/\partial x_j$ as well as coordinates x_j, then

$$\overline{H}(X, P) = \tilde{H}(X, -P), \quad (14)$$

where the tilde denotes transposition of indices of spin matrices or of arguments of any nonlocal kernel.

If the terms in (12) involving Σ_α are dropped and only the normalization constraint retained (only $\lambda_{\alpha\alpha}{}^\alpha$ nonzero) then we obtain the well-known resonance variational equations.[9-11] Our variational method may be regarded as a generalization including self-energy contributions.

In the case of degeneracies (linearly independent φ_α belonging to the same z_α) one has the usual freedom of choice. As a reasonable physical principle for resolving such arbitrariness it is natural to require that the similarity transformation commute with all constants of the motion. Under fairly general conditions it can be shown[18] that Eqs. (12) and (5) and this additional requirement are satisfied by $\overline{\varphi}_\alpha = \varphi_{\overline{\alpha}}$, where the quantum-number set $\overline{\alpha}$ differs from α only by reversal of those quantum numbers odd under time reversal [usually only the m of any Y_{lm} and the $\vec{k}$ of any $\exp(i\vec{k}\cdot\vec{R}_{\text{c.m.}})$]. This generalizes the standard rule[9-11]: Take the complex conjugate of Y_{lm} factors, but not of radial wave functions or multiplicative c-number factors.

The connection with time reversal is clarified by consideration of the relation between the in states and the out states. The T-matrix elements in Fock-Tani representation are[14,19]

$$T_{\beta\alpha} = (\overline{\varphi}_\beta|\hat{T}|\varphi_\alpha) = \langle 0|\hat{a}_\beta\hat{T}\hat{a}_\alpha{}^\dagger|0\rangle = (\overline{\varphi}_\beta|\hat{V}|\psi_\alpha{}^+) = (\overline{\psi}_\beta{}^-|\hat{V}|\varphi_\alpha). \quad (15)$$

Here $|\psi_\alpha{}^+)$ and $(\overline{\psi}_\beta{}^-|$ are solutions of the in-state and out-state Lippmann-Schwinger equations, respectively. Recalling $\hat{T} = \hat{S}^{-1}\hat{T}_{\text{Fock}}\hat{S}$ and using (7) gives

$$T_{\beta\alpha} = \langle 0|\hat{B}_\beta\hat{T}_{\text{Fock}}\hat{A}_\alpha{}^\dagger|0\rangle. \quad (16)$$

Thus $\hat{A}_\alpha{}^\dagger|0\rangle$, which contains φ_α, is the $t\to-\infty$ asymptotic initial state which evolves into a pure outgoing-wave decaying state $|\psi_\alpha{}^+\rangle$ representing a particle which has completely decayed by time zero, whereas $\hat{B}_\beta{}^\dagger|0\rangle$, which contains $\overline{\varphi}_\beta{}^*$, describes the asymptotic final $(t\to\infty)$ "antidecaying" state from which the pure incoming-wave state $|\overline{\psi}_\beta{}^-\rangle$ at $t=0$ is "retroevolved."[20] This agrees with the conclusions of Baker[21] (compare also the analysis of Bohm[8]).

We conclude by examining the explicit form of Eqs. (12) and their solution in the simplest case of a single particle in a local potential.[18] Assuming $H(x) = -\frac{1}{2}\nabla^2 + V(x)$, one can evaluate Σ_α to second order in the decay interaction using the Liouville-space representation[17] and the explicit Fock-Tani Hamiltonian.[22] In the case of a single resonance state,

$$\Sigma_\alpha = \int \overline{\varphi}_\alpha(x)[H(x)-\epsilon_\alpha]G_\alpha(x,y)[H(y)-\epsilon_\alpha]\varphi_\alpha(y)dx\,dy$$
$$= -\int\overline{\varphi}_\alpha(x)[-\tfrac{1}{2}\nabla^2 + 2V(x) - \epsilon_\alpha]\varphi_\alpha(x)dx + \int\overline{\varphi}_\alpha(x)V(x)G_\alpha(x,y)V(y)\varphi_\alpha(y)dx\,dy, \quad (17)$$

where

$$G_\alpha(x,y) = (2\pi)^{-d}\int\frac{e^{ik(x-y)}}{\epsilon_\alpha - \frac{1}{2}k^2 + i\eta}\,d^dk \quad (18)$$

and d is the number of dimensions. The first expression shows that Σ_α vanishes if φ_α is a bound state whereas the second gives, with (12),

$$-\tfrac{1}{2}(1-I_\alpha)\nabla^2\varphi_\alpha(x) - I_\alpha V(x)\varphi_\alpha(x) + V(x)\int G_\alpha(x,y)V(y)\varphi_\alpha(y)dy = (\lambda_\alpha - \epsilon_\alpha)\varphi_\alpha(x), \quad (19)$$

where $\lambda_\alpha = \lambda_{\alpha\alpha}{}^\alpha$ and

$$I_\alpha = -\int\overline{\varphi}_\alpha(x_1)V(x_1)[\partial G_\alpha(x_1,x_2)/\partial\epsilon_\alpha]V(x_2)\varphi_\alpha(x_2)dx_1\,dx_2. \quad (20)$$

One can write (19) as $D_\alpha\varphi_\alpha = \lambda_\alpha\varphi_\alpha$, where D_α is a non-Hermitian, nonlinear effective Hamiltonian. The fact that D_α is a nonlinear operator (functional of $\overline{\varphi}_\alpha$ and φ_α) even for a single particle can be interpreted as a self-interaction arising from the orthogonalization between the continuum and the decaying discrete state.[14] The complex conjugate of the second Eq. (12) is $D_\alpha{}^\dagger(\overline{\varphi}_\alpha)^* = \lambda_\alpha{}^*(\overline{\varphi}_\alpha)^*$, where $D_\alpha{}^\dagger$ is the usual Hermitian conjugate of D_α.

We have solved (19) for the case of a particle in one dimension tunneling out of a double-delta well $b[\delta(x+\frac{1}{2}) + \delta(x-\frac{1}{2})]$. The even-parity wave functions $\varphi_n(x)$ are const$\times\cos(kx)$ for $|x|<\frac{1}{2}$ and const$\times\exp(ik|x|)$ for $|x|>\frac{1}{2}$, where k has positive real part $n\pi(1-b^{-1}-b^{-2}+\dots)$ and positive imaginary part $\frac{1}{2}(n\pi)^2b^{-2}+\dots$ with $n=1,3,5,\dots$. The odd-parity solutions ($n=2,4,6,\dots$) are similar. These solutions have nonzero current, yet decay exponentially with $|x|$ in the exterior region. The resonance parameters determined from z_α agree with those calculated from the transmission coefficient with use of the scattering eigenstates.[18] The dual states are $\overline{\varphi}_n = \varphi_n$ since n is invariant under time reversal.

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[1]G. Gamow, Z. Phys. 51, 204 (1928).

[2]A. J. F. Siegert, Phys. Rev. 56, 750 (1939).

[3]P. L. Kapur and R. E. Peierls, Proc. Roy. Soc. London, Ser. A 166, 277 (1938).

[4]J. Aguilar and J. M. Combes, Commun. Math. Phys. 22, 269 (1971).

[5]E. Balslev and J. M. Combes, Commun. Math. Phys. 22, 280 (1971).

[6]B. R. Junker, Phys. Rev. Lett. 44, 1487 (1980).

[7]B. R. Junker, in *Advances in Atomic and Molecular Physics*, edited by D. Bates and B. Bederson (Academic, New York, 1982), Vol. 18, pp. 207 ff. This article gives a review of previous work.

[8]A. Bohm, J. Math. Phys. 21, 1040 (1980), and 22, 2813 (1981).

[9]A. Herzenberg and F. Mandl, Proc. Roy. Soc. London, Ser. A 274, 253 (1963).

[10]J. N. Bardsley and B. R. Junker, J. Phys. B 5, L178 (1972).

[11]R. A. Bain, J. N. Bardsley, B. R. Junker, and C. V. Sukumar, J. Phys. B 7, 2189 (1974).

[12]The word "particle" is used here in a general sense in connection with either tunneling of a single particle out of a well or decay of a composite particle.

[13]For an earlier version, see M. D. Girardeau, in *Recent Progress in Many-Body Theories*, edited by J. G. Zabolitzky, M. de Llano, M. Fortes, and J. W. Clark, Lecture Notes in Physics Vol. 142 (Springer-Verlag, Berlin, 1981), pp. 355 ff, and Bull. Am. Phys. Soc. 28, 782 (1983).

[14]For a review and references to the original literature, see M. D. Girardeau, Int. J. Quantum. Chem. 17, 25 (1980). See also E. Ficocelli Varrachio and M. D. Girardeau, J. Phys. B 16, 1097 (1983).

[15]R. Fleckinger and Y. Soulet, Physica (Utrecht) 119A, 243 (1983).

[16]We assume that the constituents of φ_α are distinguishable; otherwise appropriate normalization factors should be included in $\hat{A}_\alpha^\dagger$ and $\hat{B}_\alpha$.

[17]M. D. Girardeau, Phys. Rev. A 28, 1056 (1983); M. D. Girardeau and C. F. Hart, Phys. Rev. A 28, 1072 (1983).

[18]C. F. Hart and M. D. Girardeau, to be published.

[19]Only the simplest case is written in Eq. (15). In general there will be several $\hat{a}^\dagger$ on the right and several $\hat{a}$ on the left, as well as $\hat{\psi}^\dagger$ and $\hat{\psi}$ operators for free constituents. Furthermore, different $\hat{a}^\dagger$ and $\hat{a}$ may correspond to different arrangement channels (see Ref. 14). The general argument is, however, the same as in the simplest case (15).

[20]We assume that the entire interaction Hamiltonian $\hat{V}$, including the dissociation (decay) and recombination terms, is adiabatically switched off as $t \to \pm\infty$. These terms occur explicitly in the Fock-Tani $\hat{V}$ whereas internal binding is in $\hat{H}_0$ (not switched off); see Ref. 14. The association of *outgoing* spherical waves (decay) with the *in* state and of *incoming* spherical waves ("antidecay") with the *out* state is standard; see any reference on scattering theory. The use of such a T-matrix element is justified when the relevant decay time is long compared to the collision time.

[21]H. C. Baker, Phys. Rev. Lett. 50, 1579 (1983). Note that his projection operators P and Q, separating the subdynamics of discrete states from that of the continuum, also occur implicitly in our formalism, since our decay matrix elements contain discrete-continuum orthogonalization terms generated by the transformation $\hat{S}^{-1}\hat{H}_{\text{Fock}}\hat{S}$ (see Ref. 14).

[22]This can be evaluated as in Appendix C of M. D. Girardeau, Phys. Rev. A 26, 217 (1982).