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Electron-ion collisions at medium energies. I. L^2 basis and resonance averaging

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Treatment of the continuum spectrum of a scattering system by a discrete set of pseudostates generated by the diagonalization of the Hamiltonian in square-integrable basis functions results in spurious resonances. An energy-averaging procedure is formulated using the Stieltjes mean values for the spectral density. The connection between this L^2 basis approach to scattering problems and the stabilization method is discussed, and an improved form of the latter is derived.

I. INTRODUCTION

Electron scattering from atomic and ionic targets at intermediate energies is of current interest, not only because of its formal theoretical importance but also for applications to plasma and astrophysical research. In spite of much effort in the past, however, no single reliable theoretical procedure is yet available.[1] Difficulties at medium energies are manifold: (i) There are too many inelastic open channels to be taken into acount by any of the conventional low-energy approaches. (ii) The energy dependence of the scattering amplitude is a result of many resonances and threshold complications. (iii) The scattering energy is not high enough so that the long-range nature of the interaction and the exchange effect are negligible. Thus, attempts to extend both the low- and high-energy approaches to the medium-energy region have been only partially successful. Unlike the low-energy case, the lack of reliable and realistic model solutions to which various approximations can be compared makes it even more difficult to develop a theory in a systematic way.

During the scattering of electrons by atomic targets, many inelastic and exchange channels can couple, thus often seriously affecting the scattering amplitude.[1] This effect is conveniently approximated by including a set of square-integrable functions into the trial scattering function in a variational or a coupled-channel calculation. Of particular interest here are the Stieltjes-Tchebycheff moment method (STMM) developed recently[2] and the stabilization method[3] (SM); both these methods employ the L^2 basis set to represent the scattering function in the interaction region $\mathscr{R}$ but, apparently, the ways in which scattering information is extracted from the basis set are quite different. After a brief discussion of the STMM in Sec. II, we clarify the relationship between the two methods in Sec. III and present an improved form of the SM.

Optical potentials for low- and medium-energy scattering are also often constructed using an L^2 basis, with each of the basis states carrying a properly weighted transition strength describing the neighboring continuum states. When the basis set contains some of the open-channel components at a given energy, the optical potential thus constructed will exhibit spurious resonances. The question of energy averaging these unphysical resonances will be discussed in Sec. IV. Our main results are contained in (3.4) which connects the STMM and SM, in (3.13) for the generalization of the SM, and in (4.11) for the smoothed R-matrix elements. Equation (4.12) is an operator version of (4.11). A comparison of the STMM with the closure approximation to the resonance spectrum is given in the Appendix.

In the present paper, we consider the extension of the low-energy coupled-channel method to medium-energy scattering. For an alternate attempt to modify the high-energy approaches for medium-energy problems, we refer to Ref. 1.

II. SQUARE-INTEGRABLE BASIS AND STMM

Scattering of electrons by ionic targets is conveniently described by the reactance amplitude defined by

$$R_{fi} = \langle \Psi_f \mid V \mid \Phi_i \rangle \ , \tag{2.1}$$

where we have neglected the exchange effect for

simplicity, and where

$$(H_0-E)\Phi_{i,f}=0,\quad H_0=H-V\ ,$$
$$(H-E)\Psi_{i,f}=0\ , \tag{2.2a}$$

that is,

$$\Psi_{i,f}=\Phi_{i,f}+G_0V\Psi_{i,f}$$
$$=\Phi_{i,f}+GV\Phi_{i,f}\ . \tag{2.2b}$$

In (2.2a) and (2.2b), we have taken the standing-wave boundary conditions so that G_0 and G involve the principal-value integrations over the energy variable. Asymptotically, all functions should be Coulombic for ionic targets.

The short-range behavior of Ψ and G is of course difficult to evaluate, and the STMM employs an L^2 basis set $\{\tilde{X}_n\}$ for this purpose. It is generated by a diagonalization of the energy and normalization matrices

$$\langle\tilde{X}_n\,|\,H\,|\,\tilde{X}_m\rangle=\tilde{E}_n\delta_{nm}\ . \tag{2.3}$$

Noting that $\tilde{X}_i$ with $\tilde{E}_i=E$ will be similar to $\Psi_{\tilde{E}_i}$ in the region $\mathscr{R}$ where V is appreciable, we may set[2]

$$\Psi_{\tilde{E}_i}\approx\tilde{X}_i/\tilde{N}_i\ , \tag{2.4}$$

where $\tilde{N}_i$ is a suitably chosen normalization constant, to be discussed more fully below. Apparently, the determination of $\tilde{N}_i$ is not trivial and the STMM provides a prescription for $\tilde{N}_i$ *without* ever evaluating the continuum functions. Once $\tilde{N}_i$ is known, then (2.1) can be expressed as

$$R_{fi}=\langle Y_f\,|\,\tilde{X}_i\rangle/\tilde{N}_i,\quad Y_f\equiv V\Phi_f\ . \tag{2.5}$$

Since the set $\{\tilde{X}_i\}$ for $n=1,2,\ldots,N$ approximately spans the full spectrum of H, we have in the region $\mathscr{R}$,

$$\sum_{n=1}^{N}|\tilde{X}_n\rangle\langle\tilde{X}_n|\approx\delta(\vec{r}-\vec{r}')\ , \tag{2.6a}$$

which is to be compared with the exact closure relationship

$$\sum_{b=1}^{B_0}|X_b\rangle\langle X_b|+\int|X_{E'}\rangle\langle X_{E'}|\rho(E')dE'$$
$$=\delta(\vec{r}-\vec{r}')\ . \tag{2.6b}$$

Note that, although $|\tilde{X}_n\rangle$ at a *single* $\tilde{E}_m$ is not correctly normalized, the *sum* (2.6a) is still a good approximation to (2.6b) and will approach (2.6b) in the limit $N\to\infty$. Therefore, the smoothing of $\{\tilde{X}_n\}$ may be sensibly carried out only for a quantity which involves a sum over $\{\tilde{X}_n\}$. For this purpose, define a distribution[2]

$$dF(E)=\left[\sum_{b=1}^{B_0}f_b\delta(E_b-E)+g(E)\right]dE\ , \tag{2.7}$$

where B_0 is the total number of bound states of H (which could be infinite),

$$f_b=|\langle Y_f\,|\,X_b\rangle|^2\ ,$$
$$(H-E_b)X_b=0\quad(E_b<0) \tag{2.8}$$
$$(H-E)X_E=0\quad(E>0)$$

and

$$g(E)=\frac{df(E)}{dE}\quad\text{or}\quad g(E)=|\langle Y_f\,|\,X_E\rangle|^2\ . \tag{2.9}$$

The corresponding distribution defined on the set $\{\tilde{X}_n\}$ is

$$d\tilde{F}(E)=\sum_{n=1}^{N}\tilde{f}_n\delta(\tilde{E}_n-E)dE\ , \tag{2.10}$$

where

$$\tilde{f}_n=|\langle Y_f\,|\,\tilde{X}_n\rangle|^2\ . \tag{2.10'}$$

Integration of dF and $d\tilde{F}$ gives

$$F(E)=\int_{-\infty}^{E}dF(E')=\sum_{b=1}^{B_0}f_b(E_b)+\int_{E_{\rm th}}^{E}g(E')dE'\ , \tag{2.11}$$

where $E_{\rm th}$ is the threshold energy for the continuum spectrum of H, and

$$\tilde{F}(E)=\sum_{n=1}^{N(E)}\tilde{f}_n(\tilde{E}_n),$$
with $$\tilde{E}_n<E\quad\text{for}\quad n<N(E)\ . \tag{2.12}$$

Evidently, $\tilde{F}(E)$ is a reasonably smooth histogram which can be compared with $F(E)$, while $d\tilde{F}$ is quite distinct from dF. $\tilde{F}$ can now be used to generate $\tilde{g}(E)$, an approximation to $g(E)=dF/dE$, by taking the Stieltjes mean values,[2] as

$$\tilde{g}(E)\equiv\frac{\Delta\tilde{F}}{\Delta\tilde{E}}=\frac{1}{2}\frac{\tilde{f}_{n+1}+\tilde{f}_n}{\tilde{E}_{n+1}-\tilde{E}_n},\quad\tilde{E}_n<E<\tilde{E}_{n+1}\ . \tag{2.13}$$

Thus, the correct spectral density $g(E)$ is approxi-

mated by $\tilde{g}(E)$ *without* ever introducing the continuum function Ψ_E. Combining (2.9), (2.10′) and (2.13), we have[2]

$$\tilde{N}_i^{-1}=\left[\frac{\tilde{g}(\tilde{E}_i)}{\tilde{f}_i(\tilde{E}_i)}\right]^{1/2}=\left[\frac{1+(\tilde{f}_{i+1}/\tilde{f}_i)}{2(\tilde{E}_{i+1}-\tilde{E}_i)}\right]^{1/2}. \tag{2.14}$$

Note that, in the limit when the number of terms N in the set $\{\tilde{X}_n\}$ gets very large, $\tilde{E}_{n+1}-\tilde{E}_n$ approaches zero while $(\tilde{f}_{i+1}+\tilde{f}_i)/2\to\tilde{f}_i$, so that eventually $\tilde{N}_i\to 0$. However, in the definition of R given by (2.5), the integral involving $\tilde{X}_i$ will also approach zero in this limit $N\to\infty$, thus resulting in an indefinite form for the reactance parameter R. This situation is similar to that encountered in the stabilization method to be described in the next section. In fact, $\tilde{f}_i$ also goes to zero[2] as $N\to\infty$, but the ratio $(\tilde{f}_i/\tilde{N}_i^2)$ will approach a definite value $\tilde{g}^{1/2}$, as shown by Langhoff.[2]

III. STABILIZATION METHOD

The set $\{\tilde{X}_n\}$ generated in (2.3) contains a great deal of dynamical information of the interaction region $\mathscr{R}$, but very little of the asymptotic boundary conditions. The stabilization method[3] (SM) extracts the scattering information by projecting $\tilde{X}_n$ onto a particular channel of interest. Thus, the scattering function is written in a form

$$\Psi_f\approx\Psi_{ft}=\mathscr{S}_f+R_t\mathscr{C}_f+\sum_{n=1}^{N}c_n\tilde{X}_n\ . \tag{3.1}$$

In (3.1), both $\mathscr{S}_f$ and $\mathscr{C}_f$ satisfy the boundary conditions at the origin and asymptotically behave like Coulombic regular and irregular functions. The short-range behavior of $\mathscr{S}_f$ and $\mathscr{C}_f$ in the interaction region $\mathscr{R}$ is chosen completely arbitrarily (but of an explicit form). Then, for $E=\tilde{E}_i$, we may require that

$$\langle\tilde{X}_i\,|\,H-E\,|\,\Psi_{ft}\rangle\approx 0\ , \tag{3.2}$$

which immediately reduces to

$$R_t=-\frac{\langle\tilde{X}_i\,|\,H-\tilde{E}_i\,|\,\mathscr{S}_f\rangle}{\langle\tilde{X}_i\,|\,H-\tilde{E}_i\,|\,\mathscr{C}_f\rangle}\equiv-\frac{\mathscr{A}(\tilde{E}_i)}{\mathscr{B}(\tilde{E}_i)}\ . \tag{3.3}$$

Comparing (3.3) with (2.5) by setting $\Phi_f=\mathscr{S}_f$, we have

$$\tilde{N}_i=-\langle\tilde{X}_i\,|\,H-E\,|\,\mathscr{C}_f\rangle\,|_{\tilde{E}_i}=-\mathscr{B}(E)\,|_{\tilde{E}_i}\ , \tag{3.4}$$

and with (2.10a)

$$\tilde{f}_i=|\,\mathscr{A}\,|^2_{E=\tilde{E}_i}\ . \tag{3.5}$$

As expected, the normalization constant $\tilde{N}_i$ indeed is related to the asymptotic boundary condition. This establishes the connection between the SM and STMM of Sec. II, which in turn suggests that the instability[3] of the SM may also be present in the STMM. Consider the behavior of $\mathscr{A}$ and $\mathscr{B}$ for large N. Since the short-range behavior of $\mathscr{S}_f$ and $\mathscr{C}_f$ are chosen arbitrarily, we may set, in the region $\mathscr{R}$,

$$\mathscr{S}_f\simeq\sum_n^N a_n\tilde{X}_n\ \text{ and }\ \mathscr{C}_f\simeq\sum_n^N b_n\tilde{X}_n\ . \tag{3.6}$$

Then, as $N\to\infty$,

$$\begin{aligned}\mathscr{A}&=\langle\tilde{X}_i\,|\,H-E\,|\,\mathscr{S}_f\rangle\,|_{\tilde{E}_i}\approx 0\ ,\\ \mathscr{B}&=\langle\tilde{X}_i\,|\,H-E\,|\,\mathscr{C}_f\rangle\,|_{\tilde{E}_i}\approx 0\ ,\end{aligned} \tag{3.7}$$

which is the origin of instability in the SM. $\mathscr{A}$ and $\mathscr{B}$ are in turn related to $\tilde{f}_i$ and $\tilde{N}_i$ so that we expect[4,5] a similar instability to appear in the STMM.

An obvious improvement of the SM and STMM may be to expand $\mathscr{A}$ in a Taylor series around $\tilde{E}_i$, as

$$\mathscr{A}(E)=\mathscr{A}(\tilde{E}_i)+(E-\tilde{E}_i)\left[\frac{d\mathscr{A}}{dE}\right]_{\tilde{E}_i}+\cdots\ , \tag{3.8}$$

where

$$\left[\frac{d\mathscr{A}}{dE}\right]_{\tilde{E}_i}=-\langle\tilde{X}_i\,|\,\mathscr{S}_f\rangle\,|_{\tilde{E}_i}+\left\langle\tilde{X}_i\left|H-E\right|\frac{\partial\mathscr{S}_f}{\partial E}\right\rangle\Bigg|_{\tilde{E}_i}\ , \tag{3.9}$$

and similarly for $\mathscr{B}$. From a practical point of view, it is important to know when the leading terms in the expansion of $\mathscr{A}$ and $\mathscr{B}$ are sufficiently small compared with the terms proportional to $(E-\tilde{E}_i)$. When $\mathscr{A}(\tilde{E}_i)$ and $\mathscr{B}(\tilde{E}_i)$ are very small, however, it is possible to adjust the parameters in $\mathscr{S}_f$ and $\mathscr{C}_f$ such that these terms are idenically zero. [As an alternative, we can[3] increase N in (3.1), which then results in shifts in $\tilde{E}_i$ and $\tilde{X}_i$ such that $\mathscr{A}$ and $\mathscr{B}$ no longer vanish.] Then, with

$$\mathscr{A}(\tilde{E}_i)=0=\mathscr{B}(\tilde{E}_i)\ , \tag{3.10}$$

we have

$$R_t=-\frac{\left[\frac{d\mathscr{A}}{dE}\right]_{\tilde{E}_i}+c_i}{\left[\frac{d\mathscr{B}}{dE}\right]_{\tilde{E}_i}} . \tag{3.11}$$

In (3.11), we explicitly retained the c_i coming from the last sum in (3.1) as this term can be quite important. However, (3.11) can be further simplified by requiring that

$$\langle \tilde{X}_i \mid \mathscr{S}_f\rangle=0=\langle \tilde{X}_i \mid \mathscr{C}_f\rangle . \tag{3.12}$$

Then $c_i^{-1}=\tilde{N}_i$ from (2.4), and

$$R_t=-\frac{\left\langle \tilde{X}_i\left|H-E\right|\frac{\partial \mathscr{S}_f}{\partial E}\right\rangle_{\tilde{E}_i}+\tilde{N}_i^{-1}}{\left\langle \tilde{X}_i\left|H-E\right|\frac{\partial \mathscr{C}_f}{\partial E}\right\rangle_{\tilde{E}_i}} , \tag{3.13}$$

where (3.10) and (3.12) are imposed on $\mathscr{S}_f$ and $\mathscr{C}_f$. In (3.13), the normalization constant $\tilde{N}_i$ is assumed to be nonzero and should be obtained by the method of Sec. II.

IV. RESONANCE AVERAGING

Comprehensive treatment of low-energy electron scattering may be given in terms of the coupled-channel method (CCM), in which strongly coupled channels are explicitly included in the wave function

$$\Psi\approx\Psi_t=\sum_{c=1}^{c_0}\psi_c u_c+\sum_{n=1}^{N}c_n\tilde{X}_n$$

$$\equiv P\Psi_t+Q\Psi_t , \tag{4.1}$$

where we have neglected for simplicity the antisymmetrization of the incoming electron with the target electrons, and the ψ_c denote the target states. The last sum contains the pseudostates which simulate the neglected channels. At low energies, where only a few channels are open, the projection P can span *all* the open channels while $Q\Psi_t$ describes the closed-channel effect, including possible true resonances. On the other hand, at higher energies where more channels become open, $Q\Psi_t$ will necessarily contain open channels and may give rise to spurious resonances which are eventually to be averaged over. To examine this problem, we write the coupled equations for $P\Psi_t$

$$P(H-E+VG_t^{Q}V)P\Psi_t=0 , \tag{4.2}$$

where

$$G_t^{Q}=\sum_{n}^{N}\mid \tilde{X}_n\rangle\frac{1}{E-\tilde{E}_n}\langle \tilde{X}_n\mid , \tag{4.3}$$

is a variational approximation to the exact $G^{Q}=[Q(E-H)Q]^{-1}$. Here and in (4.1), we simply assume that $\tilde{X}_n$ are in the Q space orthogonal to P. Obviously, G_t^{Q} will have singularities at $E=\tilde{E}_n$, some of which give rise to true physical resonances, while others are spurious if the Q space contains open channels. We write the exact reactance matrix as

$$R=R^{P}+R^{Q} , \tag{4.4}$$

where

$$R^{P}\equiv\langle P\Psi^{P}\mid V\mid P\Phi\rangle , \tag{4.5a}$$

$$R^{Q}\equiv\langle P\Psi^{P}\mid VG^{Q}V\mid P\Psi\rangle , \tag{4.5b}$$

with

$$\begin{aligned}&(H_0-E)P\Phi=0,\quad P(H-E)P\Psi^{P}=0 ,\\ &Q(H-E)QG^{Q}Q=-Q .\end{aligned} \tag{4.6}$$

R^{Q} of (4.5b) may be written in a slightly different but more symmetric form

$$R^{Q}=\langle P\Psi^{P}\mid V\mathscr{G}^{Q}V\mid P\Psi^{P}\rangle , \tag{4.7}$$

where

$$\mathscr{G}^{Q}=[Q(E-H-VG^{P}V)Q]^{-1} ,$$

$$G^{P}=[P(E-H)P]^{-1} .$$

The shift operator $VG^{P}V$ in $\mathscr{G}^{Q}$ does not change the main discussion below so that we will simply neglect it here. Then, using (4.3) we have

$$R^{Q}\approx R_t^{Q}=\sum_{n}^{N}\mid\langle Y^{P}\mid\tilde{X}_n\rangle\mid^2/(E-\tilde{E}_n) , \tag{4.8}$$

where $Y^{P}\equiv VP\Psi^{P}$. Incidentally, note that, when $P\Psi_t$ contains *all* the open channels, $E<\tilde{E}_n$ for almost all $\tilde{E}_n$ and we have the bound on R^{Q} given by R_t^{Q} in accordance with the minimum principle.[6]

For medium energies where the singularities in (4.8) are spurious, R_t^{Q} requires averaging. Burke *et al.*[7] have recently studied the applicability of the I-averaging procedure originally developed for the nuclear optical potential. (For this purpose, it is more convenient to consider the T matrix). Based on the consideration of the previous sections, we examine here an alternate procedure. We immediately identify $\mid\langle Y^{P}\mid\tilde{X}_n\rangle\mid^2$ with $\tilde{f}_n$ of (2.10′), and set

$$\widetilde{F}\equiv\sum_{n=1}^{N(E)}\widetilde{f}_n\equiv\sum_{n=1}^{N(E)}|\langle Y^P|\widetilde{X}_n\rangle|^2\underset{\substack{E\to\infty\\N\to\infty}}{\to}\langle Y^P|Q|Y^P\rangle\ , \tag{4.9}$$

which is equivalent to $\widetilde{F}$ of (2.12). Thus, we can readily obtain the mean values

$$\widetilde{g}(E)=\frac{1}{2}\frac{\widetilde{f}_{n+1}+\widetilde{f}_n}{\widetilde{E}_{n+1}-\widetilde{E}_n},\quad \widetilde{E}_n<E<\widetilde{E}_{n+1}\ . \tag{4.10}$$

In order to apply $\widetilde{g}(E)$ to the evaluation of R_t^Q, we further fit the histograms $\widetilde{g}(E)$ by a smooth function $\bar{g}(E)$. Then, R_t^Q can be set equal to the principal-value integral

$$\bar{R}_t^Q(E)=\mathscr{P}\int_{-\infty}^{\infty}dE'\bar{g}(E')/(E-E')\ , \tag{4.11}$$

which is a perfectly *smooth function* of E. In addition to the convergence of the procedure (4.10) as $N\to\infty$, we have here the powerful constraints (4.9).

It is also possible to obtain a smooth optical potential by directly examining the *operator* VG_t^QV in (4.2). The procedure is quite similar to the above, and we obtain

$$PV\bar{G}_t^QVP=\sum_{n=1}^{N}\mathscr{P}\int_{\widetilde{E}_n}^{\widetilde{E}_{n+1}}\left[\frac{PV\bar{Q}_nVP}{\widetilde{E}_{n+1}-\widetilde{E}_n}\right]\frac{dE'}{E-E'}\ , \tag{4.12}$$

where

$$\bar{Q}_n(E')=\overline{\tfrac{1}{2}(\widetilde{Q}_{n+1}+\widetilde{Q}_n)},\quad \widetilde{Q}_n\equiv|\widetilde{X}_n\rangle\langle\widetilde{X}_n|\ , \tag{4.13}$$

and the bar denotes a suitable smoothing of the histogram operators $\widetilde{Q}_{n+1}+\widetilde{Q}_n$ which are constant if E' is in the interval $\widetilde{E}_n<E'<\widetilde{E}_{n+1}$.

The absorption effect of the Q space (which is partially open) may be recovered by unitarization, i.e., by using the Heitler equation and converting the R matrix to a T matrix. More directly, from (4.12), we may set the imaginary part of the G^Q contribution to the optical potential to

$$-i\pi\sum_{\text{open}}PV|\bar{Q}_m\Psi_m^Q\rangle\delta(E_m^Q-E)\langle\bar{Q}_m\Psi_m^Q|VP\ , \tag{4.14}$$

where the sum in (4.14) is over the open channels in the Q space.

V. DISCUSSION

At present, there exists no uniformly reliable theory for medium-energy scattering. Several approaches have been proposed[1,8,9] in recent years, but their usefulness is yet to be fully explored. As discussed above, the extension of the coupled-channel method to medium energies requires a set of pseudostates which can give rise to spurious resonances. We have given a simple procedure to average over these resonances. Applications of the results obtained here to actual physical systems would be very complicated for a complex electron-ion system, but computational difficulties seem to be within the capability of present-day computers, especially if one limits the size of the P and Q spaces and then constructs the appropriate Hamiltonian for such a system. As a sequel to this paper, we will report on the study of these questions, including the effect of radiative coupling,[10] which becomes important for heavier ions. Eventually, we plan to apply the theory to the evaluation of dielectronic recombination[11] and Auger ionization amplitudes.[12–14]

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APPENDIX

In connection with the resonance averaging procedure discussed in Sec. IV, it is of practical interest to consider the *closure* approximation on G^Q defined by (4.6) and its approximation G_t^Q given by (4.3). If we let

$$G^Q(E)\equiv\frac{1}{Q(E-H)Q}\to\frac{Q}{E-\bar{E}}\ , \tag{A1}$$

then, for a "correct" choice of $\bar{E}$ at each fixed E, we will have the correct R^Q. Of course $\bar{E}$ is not known *a priori* and Ref. 1, for example, discusses various ways to estimate this average energy.

(i) Consider an operator identity

$$\frac{1}{a}=\frac{1}{b}-\frac{1}{b+b(1/c)b}\ , \tag{A2}$$

where a and b are arbitrary operators and $c=a-b$. If we choose

$$\begin{aligned}&a=Q(E-H)Q\ ,\\ &b=Q(E-\bar{E})Q,\quad c=Q(\bar{E}-H)Q\ ,\end{aligned} \tag{A3}$$

then

$$G^{Q}=\frac{Q}{E-\bar{E}}\left[\frac{1}{1+A}\right], \tag{A4}$$

where

$$A\equiv Q\left[\frac{\bar{E}-H}{E-\bar{E}}\right]Q\ . \tag{A5}$$

An approximation to A of the form

$$A\approx A_t=\sum_n A\,|\tilde{X}_n\rangle\langle\tilde{X}_n|A\,|\tilde{X}_n\rangle^{-1}\langle\tilde{X}_n|A \tag{A6}$$

gives immediately

$$G^{Q}\to G_t^{Q}=\frac{Q}{E-\bar{E}}\left[1-\sum_n A\,|\tilde{X}_n\rangle\langle\tilde{X}_n|A+A^2|\tilde{X}_n\rangle^{-1}\langle\tilde{X}_n|A\right]. \tag{A7}$$

This form was used in obtaining a maximum principle[15] when the Q space is completely closed and by a proper choice of the parameter E such that $A<0$ for all $E<\bar{E}$.

The second term in (A7) corrects for the simple closure approximation represented by the first term. For a large enough set $\{\tilde{X}_n\}$, G_t^{Q} should become insensitive to the choice of $\bar{E}$. We also note that (A7) does not seem to have the obvious singularity structure of the original G_t^{Q}. Therefore, $\bar{E}$ may be chosen such that E-$\bar{E}$ is not too small and yet the second term in (A7) is kept small.

(ii) An alternative choice for b in (A2) is

$$\begin{aligned} b&=Q(\bar{E}-H)Q\ ,\\ c&=Q(E-\bar{E})Q\ , \end{aligned} \tag{A8}$$

which results in

$$G^{Q}=\frac{1}{Q(\bar{E}-H)Q}-\frac{1}{Q(\bar{E}-H)Q+\dfrac{[Q(\bar{E}-H)Q]^2}{E-\bar{E}}}\ , \tag{A9}$$

and thus

$$\begin{aligned} G^{Q}\to G_t^{Q}=&\sum_n |\tilde{X}_n\rangle\langle\tilde{X}|\bar{E}-H|\tilde{X}_n\rangle^{-1}\langle\tilde{X}_n|\\ &-\sum_n |\tilde{X}_n\rangle\left\langle\tilde{X}_n\left|Q(\tilde{E}-H)Q+\frac{[Q(E-\bar{H})Q]^2}{E-\bar{E}}\right|\tilde{X}_n\right\rangle^{-1}\langle\tilde{X}_n|\ . \end{aligned} \tag{A10}$$

Again, (A10) may be made *not* to blow up at E by choosing a proper $\bar{E}$, since the final result should not be too sensitive to $\bar{E}$ so long as enough terms are included in the set $\{\tilde{X}_n\}$. It should be stressed that, although (A7) and (A10) are similar in form, they are two quite distinct approximations.

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