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A NOTE ON THE CONSTRUCTION OF PROJECTION OPERATORS IN THE SEMI-CLASSICAL APPROXIMATION

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ABSTRACT

The projection operators onto various subsets of states of a quantum mechanical system are constructed in a semi-classical approximation based on the Wigner transformation of statistical mechanics. As illustrations, explicit operator expressions are derived for the cases of central Coulomb potential, one-dimensional harmonic oscillator, and the radial Coulombic states of specified angular momenta. Accuracy of these operators is then examined in some detail in terms of the overlap integrals and dipole transition probabilities. The semi-classical approximation is found to be effective in the energy regions away from the classical turning points. Extensions of the approach to partially projected Green's functions and other related moments are discussed and their applications to scattering problems pointed out.

I. INTRODUCTION

Projection operators occur frequently in formulations of theories of scattering reactions, such as that of Feshbach and its subsequent developments. For example, a calculation of compound resonance states may be set up in terms of the closed channel operator $Q$ which is orthogonal to all open channels at a given energy $E$. The variational bound formulation of effective potentials and resulting bounds on reaction matrix elements is also developed with the use of projection operators.

The difficulty of constructing such projection operators has been an obstacle in the application of these theories. In this paper we describe the use of the Wigner transformation of statistical mechanics to provide a semi-classical approximation for projection operators.

The Wigner transformation expresses the Boltzmann function as a certain Fourier transform of the quantum mechanical density matrix. Applied to the case of the single particle distribution function this relation is

$$ f(\vec{x}, \vec{p}) = \frac{1}{2\pi\hbar^3} \int \left( \frac{\vec{x} - \vec{p}}{2} \mid \vec{p} + \frac{\vec{p}}{2} \right) \exp\left[i\vec{p} \cdot \vec{x}/\hbar\right] d^3r \quad (1.1) $$

Here $f$ is the Boltzmann function for a particle at $\vec{x}$ with momentum $\vec{p}$ and $(\vec{x} \mid \rho \mid \vec{y})$ is the density matrix in a coordinate space representation. The inverse of (1.1) is

$$ \rho(\vec{x}, \vec{y}) = \frac{1}{\hbar} \int d^3p \left( \frac{i}{\hbar} \frac{\vec{x} + \vec{p}}{2} \right) \exp\left[i\vec{p} \cdot \left(\vec{x} - \vec{y}\right)/\hbar\right]. \quad (1.2) $$

The normalization in Eq. (1.1) is so chosen that

$$ \int f(\vec{x}, \vec{p}) d^3x d^3p = \int d^3x (\rho(\vec{x}) \mid \vec{x}) = 1 \quad (1.3) $$
when $p$ is expressed in a Hilbert space representation:

$$
(x|p|y) = \frac{1}{M} \sum_{\alpha=1}^{M} \psi_{\alpha}(x) \psi_{\alpha}^{*}(y),
$$

(1.4)

the average being over an appropriate ensemble with $\psi_{\alpha}$ the wave function of $\alpha$ in that ensemble.

II. PROJECTION OPERATOR ONTO STATES OF ONE OR MORE PARTICLES

Relations (1.1), (1.2), and (1.4) suggest the application to projection operator construction with a change in normalization, of course. Consider a complete set $\chi_{\lambda}(x)$ of orthonormal single particle wave function. The projection operator onto a subset $\mathcal{J}$ of these is

$$
(x|\Lambda|y) = \sum_{J} \chi_{\lambda}(x) \chi_{\lambda}^{*}(y).
$$

(2.1)

A classical phase space function $F(x,p)$ is introduced as

$$
F(x,p) = \int \left( \frac{p}{\hbar} x + \frac{1}{2} p^{2} \right) \exp[i \mathbf{x} \cdot \mathbf{p}] d^{3}x.
$$

(2.2)

The inverse transformation is

$$
(x|\Lambda|y) = \frac{1}{\hbar^{3}} \int \frac{F(x,y)}{\mathcal{J}} \exp[i \mathbf{x} \cdot \mathbf{p}] d^{3}x.
$$

(2.3)

If the $\chi_{\lambda}$ are normalized to unity, the normalization of $F$ is

$$
\int F(x,p) d^{3}x d^{3}p = h^{3} \sum_{J}.
$$

(2.4)

Consider now the plane wave states

$$
\psi_{p}(x) = \frac{1}{\sqrt{\mathcal{V}}} \exp[i \mathbf{p} \cdot \mathbf{x}]
$$

in some large volume $\mathcal{V}$. The projection operator onto states of momentum less than $P$ is

$$
(x|\Lambda|y) = h^{-3} \int_{p<P} d^{3}p \exp[i (\mathbf{x} - \mathbf{y}) \cdot \mathbf{p}/\hbar] .
$$

(2.5)

For this projection operator Eq. (2.2) gives

$$
F(x,p) = \int_{q<P} d^{3}q \delta(q - p), \text{ } x \text{ in } \mathcal{V}.
$$

(2.6)
We see that $F$ is unity in the "allowed" region ($p < P$) of phase space and vanishes outside this region.

The above suggests the following approximate model for a projection operator. Define

$$F(\vec{x}', p) = 1,$$

with $(\vec{x}', p)$ in a region $\mathcal{R}$ of classical phase space, and

$$F(\vec{x}', p) = 0, \quad (\vec{x}', p) \not\in \mathcal{R}.$$  \hspace{1cm} (2.7)

Then the quantum mechanical projection operator corresponding to the classical phase space $\mathcal{R}$ is

$$(\vec{x} | \Lambda | \vec{y}) = \hbar^{-3} \int d^3p \exp[ip \cdot (\vec{x} - \vec{y})/\hbar],$$

with $(\vec{x}', p)$ in $\mathcal{R}$. \hspace{1cm} (2.8)

The generalization to the case of $N$ particles is obvious.

Let $F(\vec{x}_1, p_1, \ldots, \vec{x}_N, p_N)$ be unity in a region $\mathcal{R}$ of the $N$-particle phase space and let $F$ vanish outside this region. Then the corresponding projection operator is

$$(\vec{x}_1, \ldots, \vec{x}_N | \Lambda | \vec{y}_1, \ldots, \vec{y}_N) = \hbar^{-3N} \int d^3p_1 \cdots d^3p_N \int d^3x \cdots d^3x' \exp \left[ i \sum_{j=1}^N \vec{p}_j \cdot (\vec{x}_j - \vec{y}_j)/\hbar \right].$$

The case of a particle in a spherically symmetric attractive potential $V(r)$ is very simple. Suppose $V(r)$ approaches zero as $r \to \infty$. Then choose

$$F(\vec{x}', p) = 1 \text{ for } \frac{p^2}{2m} + V(r) \leq E \leq 0,$$

$$= 0 \text{ otherwise.}$$  \hspace{1cm} (2.9)

Let

$$P(x) = \left[ 2m \left( E - V(x) \right) \right]^{1/2}.$$  \hspace{1cm} (2.11)

[We are to set $P = 0$ if the right-hand side of (2.11) is imaginary.] The expression (2.8) then gives us

$$(\vec{x} | \Lambda | \vec{y}) = \frac{1}{2\pi^2 |\vec{x} - \vec{y}|^3} [\sin \theta - \theta \cos \theta],$$

with $(\vec{x}, p)$ and $(\vec{y}, p)$ in $\mathcal{R}$. \hspace{1cm} (2.12)

The projection operator onto all bound states of a Coulomb potential, for example,

$$V(r) = -\frac{2n^2}{r}$$

is then [now $E = 0$ in Eq. (2.11)]

$$(\vec{x} | \Lambda_B | \vec{y}) = \left[ 2\pi^2 (a_0 |\vec{x} + \vec{y}|/(2\pi))^{3/2} \right]^{-1} 
\times \left[ \sin \theta - \theta \cos \theta \right],$$

$$G = \left[ |\vec{x} - \vec{y}|^3/(2\pi^2 (a_0 |\vec{x} + \vec{y}|))^{3/2} \right],$$

where $a_0$ is the Bohr radius.

The projection operator onto the continuum of the Coulomb states is, in the present approximation, obtained as follows:

$$P_C = 1 - F,$$

so

$$(\vec{x} | \Lambda_C | \vec{y}) = 8(\vec{x} - \vec{y}) - (\vec{x} | \Lambda_B | \vec{y}).$$  \hspace{1cm} (2.14)
The relation (2.14) is of course exact. This results from the fact that if \( F = 1 \) on all phase space our approximation gives the exact result

\[
\langle \vec{x}|A|\vec{y} \rangle = \delta(\vec{x} - \vec{y}).
\]  

(2.15)

We emphasize that the expressions (2.12) and (2.13) are defined only in that domain of \( \vec{x} \) and \( \vec{y} \) for which \( F((\vec{x} + \vec{y})/2) \) is real. Thus \( \langle \vec{x}|A|\vec{y} \rangle \) vanishes for \( (\vec{x} + \vec{y})/2 \) outside the classical turning points. Extension of our procedure into the classically forbidden regime appears possible (as in the WKB method), but is not discussed here.

The formal relation

\[
A^2 = A
\]  

(2.16)

to be satisfied by projection operators is not satisfied exactly by the approximation (2.8). As the domain \( \mathcal{R} \) becomes large compared with \( \Phi^3 \)--the semi-classical limit--it is easily seen that (2.16) becomes valid, however. For the classical phase space \( \mathcal{R} \) described by the symmetric variable \( (\vec{x} + \vec{y})/2 \), the operator given by (2.8) is hermitian.

The expression corresponding to (2.3) when a momentum space representation is used is

\[
\langle \vec{q}|A|\vec{q}' \rangle = \hbar^{-3} \int d^3x \ d^3y \exp[i(\vec{q}' \cdot \vec{y} - \vec{q} \cdot \vec{x})] \langle \vec{x}|A|\vec{y} \rangle
\]

\[
= \hbar^{-3} \int d^3r \ F(\vec{r},(\vec{q} + \vec{q}')/2) \exp[i(\vec{q}' - \vec{q}) \cdot \vec{r}] .
\]  

(2.17)

It is also of interest to consider the applications of (2.5) and (2.9) to collision problems. For scatterings in which all the states in the set \( \mathcal{S} \) correspond to open channels, \( A_B \) for the states in \( \mathcal{S} \) may be used to construct the open-channel projection operators. Thus, for example, in the e-H scattering near the ionization threshold, we may use \( A_B(\vec{t};\vec{t}') \) of (2.12) and construct the operator as

\[
A_B(\vec{t},\vec{t}';\vec{t}',\vec{t}'') = A_B(\vec{t};\vec{t}') + A_B(\vec{t}';\vec{t}'')
\]

(2.18)

and its complement

\[
A_C(\vec{t},\vec{t}';\vec{t}',\vec{t}'') = 5(\vec{t} - \vec{t}') 5(\vec{t}' - \vec{t}'') - A_B(\vec{t},\vec{t}';\vec{t}',\vec{t}'') = \Lambda^Q,
\]  

(2.19)

where \([A_B(\vec{t},\vec{t}'), A_B(\vec{t}';\vec{t}'')] = 0\). These operators, which are hermitian and almost idempotent, may then be used to study the resonance structure, distortion effect, and the bounds on scattering parameters near the ionization threshold. Alternatively, a similar projection operator \( \Lambda^Q \) onto the closed-channel space \( \mathcal{Q} \) for the two-electron system may also be obtained directly from the multiparticle generalization (2.9).

The effective pseudopotential for this process can then be constructed with \( \Lambda^Q \).

Generalizations of (2.16) and (2.19) to systems involving more than two electrons are also straightforward and the result could be used with greater advantage in the e-Atomic and e-Molecular reactions, simply because \( \Lambda^P \) and \( \Lambda^Q \) are now very simple to evaluate.
III. APPLICATIONS OF COULOMB PROJECTION OPERATOR

As a first application of the projection operators derived in Sec. II, we study the ionization transitions of hydrogenic targets by fast electron impact. Since the bound state → bound state transitions are dominant in this case, the usual closure approximation to the transition probabilities leads to gross overestimate, and it is necessary to carefully isolate the continuum contributions. Thus, the relevant transition probability is given in the leading order by

\[ M_{n \ell}^C = \frac{1}{2 \ell + 1} \sum_{m} \langle n, \ell, m; \mathbf{x} | \mathbf{A}_C (\mathbf{x}, \mathbf{y}) | n, \ell, m; \mathbf{y} \rangle, \]

(3.1)

where all the dipole transitions from \( |n, \ell, m; \mathbf{x} \rangle \) to the continuum are included. Similarly, we also have

\[ M_{n \ell}^B = \frac{1}{2 \ell + 1} \sum_{m} \langle n, \ell, m; \mathbf{x} | \mathbf{A}_B (\mathbf{x}, \mathbf{y}) | n, \ell, m; \mathbf{y} \rangle \]

(3.2)

corresponding to the transitions to all the bound states.

In (3.1) and (3.2), we have denoted the hydrogenic states as

\[ |n, \ell, m; \mathbf{x} \rangle = \psi_{n \ell m}(\mathbf{x}) = R_{n \ell}(x) Y_{\ell m}(\hat{x}), \]

(3.3)

while the projection operators \( \mathbf{A}_B \) and \( \mathbf{A}_C \) are given by (2.13) and (2.14), with \( E = 0 \).

Evidently, the contribution to (3.1) coming from the \( \delta \)-function part in (2.14) corresponds to transitions to all available states, both bound and continuum, and is given in this case by

\[ M_{n \ell}^A = \frac{1}{2 \ell + 1} \sum_{m} \langle n, \ell, m; \mathbf{x} | \mathbf{x}^2 \delta (\mathbf{x} - \mathbf{y}) | n, \ell, m; \mathbf{y} \rangle \]

\[ = \frac{M_{n \ell}^B + M_{n \ell}^C}{2}, \]

(3.4)

where the quantities defined with bar denote exact values. An additional quantity of interest for our study is the overlap integral defined as

\[ S_{n \ell} = \frac{1}{2 \ell + 1} \sum_{m} \langle n, \ell, m; \mathbf{x} | \mathbf{A}_B (\mathbf{x}, \mathbf{y}) | n, \ell, m; \mathbf{y} \rangle. \]

(3.5)

Obviously, with the exact \( \mathbf{A}_B \) in (3.5), in place of the approximate form (2.13), we expect that

\[ S_{n \ell} = 1, \text{ for the } n \text{th state in } \mathbf{A}_B \]

(3.6)

\[ = 0 \text{ otherwise.} \]

The exact values of \( M_{n \ell}^B \) and \( M_{n \ell}^C \) are also available for \( n \leq 4 \) for ready comparison.

More explicitly, after the sum over the magnetic quantum numbers is carried out, \( M_{n \ell}^B \) becomes

\[ M_{n \ell}^B = \frac{1}{\pi} \int_0^\infty x^2 dx \int_0^\infty y^2 dy \int_{-1}^1 d\mu P_{\ell}(\mu) \mu \times \left[ \sin G - G \cos G \right]. \]

(3.7)

For some values of \( \mu \) in the range \( |\mu| < 1 \), the variable \( v \) goes through zeros and thus \( G \) becomes singular. This causes the integrand
in (3.9) to oscillate violently and makes the $du$ integration difficult. To avoid this problem in the actual numerical integration, we change the variables $(x, y)$ to $(\tilde{x}, \tilde{y})$, where $\tilde{t} = \tilde{x} + \tilde{y}$, and rewrite the $M_{n\ell}^B$ in the form

$$M_{n\ell}^B = \frac{1}{\pi} \int_0^\infty x^2 \, dx \int_0^\infty t^2 \, dt \, R_{n\ell}(x) \int_{-1}^{1} R_{n\ell}(b) \frac{1}{d^3} \sin G \, G \cos G \, X \, (t \alpha - x) \, P_\delta(\mu) \, d\alpha,$$

(3.8)

where

$$d = [4x^2 + t^2 - 4xt\alpha]^2$$

$$b = [t^2 + x^2 - 2xt\alpha]^2$$

$$G = 2d/(t)^{1/2}$$

$$\mu = (t \alpha - x)/b.$$  

The form (3.8) and the corresponding expression for $S_{n\ell}$ were used in the actual numerical calculations, and the result is given in Table I for the cases $n = 1, 2, 3$ and $\ell = 0$. A semi-analytic integration formula, which is useful for rapidly oscillating integrands, and the Newton-Cotes five-point formulas with varying mesh sizes are used to ascertain the accuracy of the triple integrations in (3.8). The actual values given in the table are obtained by rough extrapolations to the limit of zero mesh sizes (Fig. 1). The mesh size $h$ is defined here by $h = 2/K_{\max}$; the convergence was found to be extremely slow, and becomes worse as $n$ was increased, especially in the $d\alpha$ integration of (3.8).

We have encountered additional difficulties in the evaluation of $M_{n\ell}^C$, because of the severe cancellation between $M_{n\ell}^A$ and $M_{n\ell}^B$ for $n > 1$, where $M_{n\ell}^A = M_{n\ell}^B \gg M_{n\ell}^C$. This seems to be a peculiarity of the Coulomb problem under consideration. The difficulty could in principle be avoided by defining $A_C$ directly in a form similar to (2.8), rather than through $A_B$ as we have done in (2.14). When the order of integrations $d^3p$ and $du$ are interchanged, the resulting integral is then well-defined. However, we are left with four dimensional integrations which are difficult to carry out numerically. For the case $n = 1$ and $\ell = 0$, we obtain $M_{10}^C = 1.1 \pm 0.2$. 
IV. PROJECTION OPERATOR IN ONE-DIMENSION (HARMONIC OSCILLATOR)

We consider in this section a one-dimensional harmonic oscillator model. Aside from the simplification in the numerical analysis, the model involves a very simple dipole coupling scheme and also allows us to study the accuracy of \( \Lambda_B \) near the classical turning point.

The parameters of the model are defined in the units

\[ m = \pi = 1, \]  

by

\[ \frac{d^2 \varphi_n}{dx^2} + a^2 x^2 \varphi_n = E_n \varphi_n, \]  

with

\[ E_n = (2n + 1)a, \quad n = 0, 1, 2, \ldots \]

\[ \varphi_n(x) = \Lambda_n H_n[(a^{\frac{1}{2}}x)] \exp(-\frac{1}{2}ax^2) \]

and

\[ \int_{-\infty}^{\infty} |\varphi_n(x)|^2 dx = 1. \]

The dipole coupling produces

\[ \left[ \int_{-\infty}^{\infty} \varphi_n^*(x) \varphi_n(x) \, dx \right]^2 = \begin{cases} \frac{n + 1}{2a} = \overline{\Lambda}_{n,n+1}, & \text{for } m = n + 1 \\ \frac{n}{2a} = \overline{\Lambda}_{n,n-1}, & \text{for } m = n - 1 \\ 0, & \text{otherwise.} \end{cases} \]

We let

\[ \overline{\Lambda}_n = \overline{\Lambda}_{n,n+1} + \overline{\Lambda}_{n,n-1} = \frac{2n + 1}{2a}. \]

The operator \( \Lambda_B \) which projects onto all the states with energy \( E_n \leq E_C \) is

\[ (x|\Lambda_B|y) = \sum_{E_n \leq E_C} \varphi_n(x) \varphi_n^*(y). \]  

The one-dimensional analogue of (2.8) gives us the semi-classical approximation to (4.5)

\[ (x|\Lambda_B|y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dp \, e^{ip(x-y)} \]

\[ = \frac{1}{2\pi} \left[ \sin(\pi u)/u \pm \sin(2\pi v)/(2v) \right]. \]

Here

\[ P^2(v) = 2E_C - a^2 v^2. \]

and

\[ u = x - y, \quad v = (x + y)/2. \]

In addition to (4.6) we define

\[ (x|\Lambda_B^+|y) = \begin{cases} \frac{1}{2\pi} \int_{-\pi}^{\pi} dp \cos(px) \cos(py), & \text{even} \\ \frac{1}{2\pi} \int_{-\pi}^{\pi} dp \sin(px) \sin(py), & \text{odd} \end{cases} \]

\[ = \frac{1}{2\pi} \left[ \sin(\pi u)/u \pm \sin(2\pi v)/(2v) \right]. \]
We note that $\Lambda_B^\pm$ and $\Lambda_B^\mp$ vanish for $|v| > v_C$, where
\[ v_C = (2\varepsilon_C/a)^{1/2}. \] (4.10)

The quantities $\Lambda_B^\pm$ would represent projection operators onto even (odd) states, corresponding to even (odd) $n$-values, except for the wrong symmetry of Eqs. (4.7) and (4.8). We shall see, however, that for those cases considered below $\Lambda_B^\pm$ represent very good approximations to the projection operators on even (odd) states.

The quantities of interest are defined by
\[ M_n^A = (n,x|x^2|x,n) \] (4.11)
\[ M_n^B = (n,x|x\Lambda_y|n,y) \] (4.12)
\[ M_n^C = M_n^A - M_n^B \] (4.13)
\[ S_n = (n,x|\Lambda_B|^2|n,y) \] (4.14)
and the corresponding integrals with $\Lambda_B^\pm$ in the place of $\Lambda_B$. We denote them by $M_n^{B\pm}$, $M_n^{C\pm}$, and $S_n^{\pm}$.

The dipole couple scheme of this model is very simple, and we have the exact values for comparison
\[ \bar{M}_n^A = \bar{M}_n^B \] (4.15)
\[ \bar{M}_n^C = 0 \] (4.16)
and
\[ \bar{S}_n^{\pm} = 1 \text{ or } 0, \text{ depending on the symmetry of } n \text{ and } \Lambda_B^\pm \]
\[ \bar{S}_n = 1. \]

The parameters of the model are chosen as
\[ a^2 = 0.45 \] (4.17)
\[ 2\varepsilon_C = 2n_C + 1, \text{ with } n_C = 10, \]
which in turn gives the cutoff value
\[ v_C = \left[ \frac{2(n_C + 1)^{1/2}}{a} \right] \approx 5.6. \] (4.18)

Table II contains the result of calculation for both cases in which $\Lambda_B^\pm$ and $\Lambda_B^\mp$ are used. The extra term in $\Lambda_B^\pm$ causes both $M_n^{B\pm}$ and $S_n^{\pm}$ to oscillate around their respective exact values, while the integrals with $\Lambda_B^\mp$ give smoother variations in $n$. The deviations of $M_n^{B\pm}$, $S_n^{\pm}$, $M_n^{B\pm}$, and $S_n^{\pm}$ are illustrated in Figs. 2 and 3. Also included in Table II is the overlap integral $s_n^{\pm}$ which was calculated using the wrong symmetry, that is, $\Lambda_B^+$ for the case with $n$ odd, and vice versa. Although the form of integrands in (4.9) are either symmetric or antisymmetric under $x \rightarrow -x$ (or $y \rightarrow -y$), $\Lambda_B^\pm$ itself does not have the definite symmetry because of the cutoff (4.10). However, we expect that $s_n^{\pm} = 0$ for those $n$ which are away from $n_C$, as given in the table. In fact, we have $s_n^{\pm} = S_n - S_n^{\pm}$, and the exact value would of course be $s_n^{\pm} = 0$. 
V. PROJECTION OPERATORS ONTO RADIAL WAVE FUNCTIONS

The numerical calculation of the dipole transitions of Sec. III can be simplified by the construction of projection operators onto radial states. Thus, the exact projection operator onto the bound Coulomb states corresponding to an angular momentum \( \ell \) is

\[
(r | \Lambda_B^\ell | r') = \sum_{n=\ell+1}^\infty R_n^\ell (r) R_n^\ell (r') .
\]  

(5.1)

To construct the semi-classical approximation to this, we proceed as follows:

The classical Hamiltonian for a particle with angular momentum \( L \) in a potential \( V(r) \) is

\[
\hat{H} = \frac{P^2}{2m} + \frac{L^2}{2mr^2} + V(r) ,
\]  

(5.2)

where \((p,r)\) are the canonical radial coordinate and momentum. For fixed \( L \), if the energy is to be less than \( E \), we must have the momentum \( p \) less than

\[
P(r) = (2m[E - L^2/(2mr^2) - V(r)])^{1/2} .
\]  

(5.3)

For the semi-classical approximation to \( \Lambda_B^\ell \) we then write

\[
(r | \Lambda_B^\ell | r') = \frac{2}{\pi} \int_0^\infty dp \, p^2 \, J_\ell (pr) \, J_\ell (pr') ,
\]  

(5.4)

with

\[
v = (r + r')/2, \quad u = (r - r') .
\]  

(5.5)

We note that \( \Lambda_B^\ell \) vanishes outside the classical turning points, \( v_C \), where

\[
P(v_C) = 0 .
\]  

(5.6)

It is consistent with the semi-classical approximation to use the asymptotic form of the spherical Bessel functions. This leads to

\[
(r | \Lambda_B^\ell | r') = \frac{1}{\pi r r'} [\sin (Pu)/u - (-)^\ell \sin (2Pv)/(2v)] .
\]  

(5.7)

To use this, we must relate \( L \) in Eq. (5.2) to \( \ell \). Two reasonable choices are

\[
L^2 = \ell (\ell + 1) = L_Q^2 ,
\]  

(5.8a)

or

\[
L^2 = (\ell + 1/2)^2 = L_C^2 .
\]  

(5.8b)

There is a strong temptation to drop the second term in brackets in (5.7), writing

\[
(r | \Lambda_B^\ell | r') \approx \frac{1}{\pi r r'} \sin (Pu)/u = \Lambda_B^\ell v .
\]  

(5.9)

Later, we shall compare use of both expressions with some exact results.

For the projection operator onto all the bound states of the Coulomb field we have \( E = 0 \) and \( V = -1/r \) in Eq. (5.3). [We set \( m = e = \hbar = 1 \).] Then (5.6) gives

\[
v_C = L^2/2 ,
\]  

with \( \Lambda_B^\ell \) vanishing within the centrifugal barrier defined by \( v < v_C \).
The quantity (3.2) can be reduced to the form, by performing
the angular integrations,

\[
M_{n\ell}^B = [(2\ell + 1)]^{-1} \int_0^\infty x^3 \, dx \int_0^\infty y^3 \, dy
\]

\[
\chi \, R_{n\ell}(x) \, R_{n\ell}(y) \left[ (\ell | \Lambda^\ell_B - 1 | y) + (\ell + 1)(\ell + 1 | \Lambda^{\ell+1}_B | y) \right]
\]

\[
= [(2\ell + 1)]^{-1}[\ell \, M_{n\ell}^B + (\ell + 1) \, M_{n\ell+1}^B].
\]  

(5.10)

The corresponding quantity \( M_{n\ell}^C \) is

\[
M_{n\ell}^C = M_{n\ell}^A - M_{n\ell}^B,
\]

(5.11)

where \( M_{n\ell}^A \) is given by Eq. (3.6). In general, \( M_{n\ell}^C \gg M_{n\ell}^B \), so
that we have \( M_{n\ell}^C = M_{n\ell}^C \). Finally, the normalization integral \( S_{n\ell} \),
defined by Eq. (3.7), is

\[
S_{n\ell} = \int_0^\infty x^2 \, dx \int_0^\infty y^2 \, dy \, R_{n\ell}(x) \, R_{n\ell}(y) \, (x|\Lambda^\ell_B | y).
\]

(5.12)

We can also define analogous quantities using the approximation (5.9)
and \( \Lambda^{00}_B \), and denote them as \( M_{n\ell}^{00} \), \( S_{n\ell}^{00} \), \( M_{n\ell}^{CC} \), etc.

As is clear from the above discussion, there are essentially
two ambiguities in the present case; we could choose either (5.8a) or
(5.8b) for the value of \( L^2 \) and thus the cutoff \( v_C \), and secondly we
could use either (5.7) or (5.9) for \( \Lambda_B \) (and \( \Lambda^{00}_B \)). We have
considered here all four possibilities. Table III contains the result
of calculations with \( L^2 = L_C^2 = (\ell + 1/2)^2 \) and both \( \Lambda^\ell_B \) and \( \Lambda^{\ell+1}_B \).
We thus have \( M_{n\ell}^{00} \), \( M_{n\ell}^B \), and \( M_{n\ell}^{CC} \), and \( M_{n\ell}^C \) corresponding to the

transitions \( \ell \rightarrow \ell + 1 \). The cases with \( L^2 = L_Q^2 = \ell(\ell + 1) \) are
considered in Table IV.

First of all, we should point out that, as in the three-
dimensional Coulomb case studied in Sec. III, \( M_{n\ell}^A \gg M_{n\ell}^B \gg M_{n\ell}^C \)
(Fig. 4). Therefore the accuracy of \( \Lambda_B \) and \( \Lambda^{00}_B \) should be judged
in terms of \( S_{n\ell} \) and \( M_{n\ell}^B \), rather than by looking at the small \( M_{n\ell}^C \).
Secondly, the results in Tables III and IV are not very sensitive to
the choices of \( L^2 \), so long as it is chosen judiciously. Incidentally,
the cutoff for \( v < v_C \) partially corrects for the error caused by the
use of asymptotic \( \Lambda^0_B \) in (5.7). Finally, we note that the extra term
in \( \Lambda_B \) (i.e., \( \Lambda_B - \Lambda^{00}_B \)) gives rise to small oscillations in \( M_{n\ell}^C \),
while \( \Lambda^{00}_B \) yields fairly smooth \( M_{n\ell}^{00} \).
VI. APPROXIMATION TO GREEN'S FUNCTIONS

The reasonable accuracy of the semi-classical approximation for projection operators suggests a similar application to certain other operators. In the present section we discuss the construction of partially projected Green's functions by this technique.

We introduce the "Green's function"

\[ (\tilde{x}|G_B|\tilde{y}) = \sum_{\mathcal{J}} \chi_\lambda(\tilde{x})(E - E_\lambda)^{-1} \chi_\lambda^*(\tilde{y}). \]  

(6.1)

Here the \( E_\lambda \) are eigenvalues of the energy for states \( \chi_\lambda \), members of a complete orthonormal set \( \{ \chi \} \), and the sum extends over a subset \( \mathcal{J} \) of these.

The semi-classical approximation to (6.1) may be obtained in exactly the same way as with (2.8) and (2.12). Thus, for all states with \( E_\lambda \leq E_c \) and potential \( V(x) \), we define

\[ P(v) = \left[ 2m (E_c - V(v)) \right]^{\frac{3}{2}} \]  

(6.2)

and

\[ E_\lambda \rightarrow \frac{p^2}{2m} + V(v), \]  

(6.3)

where \( v = \frac{3}{2}(\tilde{x}^2 + \tilde{y}^2) \) as before. Then, the operator \( G_B \) in the semi-classical approximation is given by

\[ (\tilde{x}|G_B|\tilde{y}) = \frac{1}{\hbar^2} \int_{P \leq P} d^3p \frac{e^{i\tilde{x}^2 \cdot \hat{p}/\hbar}}{(E_c - p^2/2m + V(v))}, \]  

(6.4)

where \( \hat{u} \equiv \tilde{x} - \tilde{y} \). After the angular integrations, (6.4) becomes

\[ \langle \tilde{x}|G_B|\tilde{y} \rangle = \frac{1}{\pi u} \int_0^{P(v)} \frac{p dp \sin(pu)}{2E_c - p^2 - 2V(v)}, \]  

(6.5)

which is the desired result. Analogously, the operator in the complementary space \( \mathcal{J} = 1 - \mathcal{J} \) can also be given directly this time as

\[ (\tilde{x}|G_C|\tilde{y}) = \frac{1}{\pi u} \int_0^{\infty} \frac{p dp \sin(pu)}{2E_c - p^2 - 2V(v)}, \]  

(6.6)

which should be convergent at large \( p \) because of the Riemann-Lebeque theorem. Of course, both \( G_B \) and \( G_C \) are defined only in the region of \( v \) such that \( P(v) \) is real.

Generalizations of (6.5) and (6.6) to operators of higher moments are obvious, as

\[ (\tilde{x}|G_B^Y|\tilde{y}) = \frac{2^{Y-1}}{\pi u} \int_0^{P(v)} \frac{p dp \sin(pu)}{[2E_c - p^2 - 2V(v)]^Y}, \]  

(6.7)

and the corresponding expression for \( G_C^Y \).

There are many possible applications of the operators (6.7); for example, the adiabatic dipole and higher multipole polarizabilities \( \alpha^Y \) may be evaluated using (6.5), while the leading nonadiabatic corrections \( \beta^Y \) to the adiabatic pseudopotentials in the low energy electron-atom collisions involve operators with \( Y = 2 \). The low-energy scattering parameters are known to be determined principally by these parameters.

The form (6.7) immediately suggests that the case with \( Y < 0 \) may also be of interest, although special care is required in the
direct evaluation of $G^-$ because of the convergence difficulties at large values of $p$. Thus, we have

$$
(x|F_B^5|y) = \frac{1}{\pi u(2)^{\frac{5}{2}}} \int_0^{P(v)} dp \sin(pu)[2E - p^2 - 2\nu]^5.
$$

(6.8)

The case with $\nu = 1$ may be used, for example, in the calculation of the partially projected oscillator strength. The main advantage of dealing with the operators in the restricted set $S$ or $\tilde{S}$ is that the contributions from each state in that set are all of the same sign, often resulting in some type of bound property.

Some insight into the nature of the approximation (6.4) can be obtained by using it to construct the actual Green's function, $G^+$, obtained by setting $P = \infty$ and using the proper retarded boundary condition.\textsuperscript{12} This gives

$$
(x|G^+|y) = -[M/(2\pi u)]\exp[iuK(v)],
$$

(6.9)

where

$$
K(v) = [2M(E - \nu(v))]^{\frac{1}{2}}.
$$

(6.10)

The corresponding expression for $G^+$ in the straight-line eikonal approximation, [which is certainly more accurate than (6.9)] is

$$
(x|G^+|y) = -[M/(2\pi u)] \exp\left[i \int_{y}^{x} K(r) \, ds(r) \right].
$$

(6.11)

Here the path integral is taken on the straight line joining points $y$ and $x$. 

We see that (6.9) corresponds to approximating the eikonal integral as

$$
\int_{y}^{x} K(r) \, ds(r) \approx |x - y| K(|x + y|/2).
$$

(6.12)
FOOTNOTES AND REFERENCES


† On sabbatical leave from the Physics Department, University of Connecticut, Storrs, Connecticut 06268. Participating guest Lawrence Berkeley Laboratory.


5. A similar expression is of course available for the case of more than one particle [see Ref. 4].


7. Planck's constant is retained in this section to explicitly exhibit classical and quantum aspects of our formulation.


13. Ref. 12, page 331.
Table II. The dipole transition probabilities $M_n$ and the overlap integrals $S_n$ for the one-dimensional harmonic oscillator model. The force constant $a^2 = 0.45$ and the cutoff energy is chosen the 10th level, with $n_C = 10$. Both cases with $A_B$ and $A_B^\dagger$ are considered.

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<tr>
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<th>$A_B$</th>
<th>$A_B^\dagger$</th>
</tr>
</thead>
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<td>$n$</td>
<td>$M_n$</td>
<td>$S_n$</td>
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<td>1.0000</td>
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<td>21.1111</td>
<td>0.8584</td>
</tr>
<tr>
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<td>0.6632</td>
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</table>

Table I. The dipole transition probabilities and the overlap integrals for the hydrogenic system, with $n = 4, 5, 6$ and $l = 0$. The full projection operator $A_B$ for bound partial wave states is used. The quantities with bar denote the exact values, in atomic units.
Table III. The hydrogenic dipole transition probabilities and overlap integrals using the radial projection operators $A_{\ell}^{\ell}$ and $B_{\ell}^{\ell}$ for the case $\ell \rightarrow \ell + 1$. The choice $L^2 = L = (\ell + \frac{1}{2})^2$ is used in the cutoff $v_C$ and momentum $P(v)$.

<table>
<thead>
<tr>
<th>$n \ell$</th>
<th>$A_{n\ell}$</th>
<th>$B_{n\ell}$</th>
<th>$C_{n\ell}$</th>
<th>$\lambda_{BO}^{n\ell}$</th>
<th>$\lambda_{CO}^{n\ell}$</th>
<th>$\lambda_{BO}^{n\ell}$</th>
<th>$\lambda_{CO}^{n\ell}$</th>
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<td>40.90</td>
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<td>0.991</td>
<td>3142.5</td>
<td>5.5</td>
<td>0.974</td>
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</table>

Table IV. The hydrogenic dipole transition probabilities and overlap integrals using the radial projection operators $A_{\ell}^{\ell}$ and $B_{\ell}^{\ell}$ for the case $\ell \rightarrow \ell + 1$. The choice $L^2 = L_Q = \ell (\ell + 1)$ is used in the cutoff $v_C$ and momentum $P(v)$.

<table>
<thead>
<tr>
<th>$n \ell$</th>
<th>$A_{n\ell}$</th>
<th>$B_{n\ell}$</th>
<th>$C_{n\ell}$</th>
<th>$\lambda_{BO}^{n\ell}$</th>
<th>$\lambda_{CO}^{n\ell}$</th>
<th>$\lambda_{BO}^{n\ell}$</th>
<th>$\lambda_{CO}^{n\ell}$</th>
</tr>
</thead>
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<tr>
<td>1 0</td>
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</table>
FIGURE CAPTIONS

Fig. 1. The convergence of the $M_{10}^{CO}$ integrations for the hydrogenic system. The angular integral in (3.8) is carried out using both the semianalytic method and the Newton-Cotes (5 point) integrations. The mesh size $h$ is defined by $h = 2/K_{max}$.

Fig. 2. The values of $M_n^B$ and $S_n$ for the one-dimensional harmonic oscillator model are given near the cutoff $n_C = 10$, where the projection operator $\Lambda_B$ is used.

Fig. 3. The values of $M_n^{B\pm}$ and $S_n^{\pm}$ for the one-dimensional harmonic oscillator model are given near the cutoff $n_C = 10$, where the projection operator $\Lambda_B^{\pm}$ is used.

Fig. 4. Variations in $n$ of the exact dipole transition probabilities of the hydrogenic system for the processes $(n,\ell) \to (\text{all states, with } \ell + 1)$, $(\text{all bound states with } \ell + 1)$, and $(\ell + 1)$. The cases with $\ell = 0$ and 1 are considered.
Hydrogen \((n=1, \ell=0)\)

- Semi-analytic
- Newton-Cotes (5-point)
- Newton-Cotes (3-point)

\[ M_{10}^{\text{c}} \]

\[ K_{\text{max}} \]

0.85 exact

Fig. 1
Fig. 3

$\Lambda_B^\pm$ with $n_c = 10$

$\overline{M}_n^{B^\pm}$

$M_n^{B^\pm}$

$\overline{S}_n^{\pm} \times 10$

$S_n^{\pm} \times 10$
Fig. 4
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