PHYSICAL REVIEW B

CONDENSED MATTER

THIRD SERIES, VOLUME 49, NUMBER 16 15 APRIL 1994-II

Accuracy of the recursion method

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(Received 21 May 1993; revised manuscript received 24 January 1994)

In this paper, the insensitivity of the projected density of states (PDOS) is investigated. Rounding errors are treated as perturbations in the recursion process when calculating the PDOS. A generalized error theory for the PDOS is developed, which includes Paige's theorem and the effects of truncation of the continued fraction. An analytic expression for the PDOS which isolates the error term is derived. This error term is shown to be exponentially insensitive to perturbations which are distant from the starting state; in contrast to eigenvalues and/or eigenfunctions which are very sensitive to small perturbations. This is what makes calculating PDOS and its integrated quantities a more stable approach compared to computing eigenvalues. This insensitivity is equivalent to a black-body theorem for the PDOS. This result is useful in practical computations because it enables an infinite system to be approximated by a particular finite one, and gives a bound on the error in the computed PDOS.

I. CALCULATING PROJECTED DENSITY OF STATES

To calculate projected quantities such as the electronic occupation of an orbital, the energy of a defect state, or the band energy and electronic occupation of a projected state, the approach is to first calculate the projected density of state (PDOS) which describes how a particular orbital couples to the entire system. The PDOS for a finite system is defined[1,2] as

$$n(u_0;E)=\sum_n |(u_0,\Psi_n)|^2\delta(E-E_n)\ , \tag{1}$$

where u_0 is the orbital of projection and Ψ_n is the eigenfunction of the system Hamiltonian with energy E_n.

The PDOS is the total density of states weighted by the probability of finding the system in a particular orbital u_0. Many quantities of physical interest can be written as integrals of the PDOS; for example: The diagonal element corresponding to u_0 of the density matrix,

$$\langle n\rangle=\int_{-\infty}^{E_F} n(u_0;E)dE\ ; \tag{2}$$

the energy expectation value for orbital u_0,

$$\langle E\rangle=\int_{-\infty}^{E_F} n(u_0;E)E\,dE\ . \tag{3}$$

Since the definition of the PDOS does not require the system to possess symmetry, this approach is applicable to amorphous or disordered solids.

In computing the PDOS, one need not solve for all the eigenfunctions and eigenvalues of the system. Calculating all eigenpairs of the Hamiltonian is impractical, both computationally and analytically, because the number of states involved in a macroscopic system is on the order of 10^{23}. Diagonalization on a computer requires a number of arithmetic operations which scales with the cube of the number of orbital degrees of freedom. Furthermore, direct diagonalization is unstable because of the sensitivity of eigenfunctions and eigenvalues to small changes in the boundary conditions. The PDOS, on the other hand, does not exhibit this sensitivity and can be computed using the recursion method[2] with fewer arithmetic operations, compared to a full diagonalization of the Hamiltonian.

This insensitivity of the PDOS with respect to the boundary conditions of the system was first pointed out by Friedel.[1] It is a black-body effect for the PDOS which Heine[2] referred to as the invariance theorem. This is similar to the black-body theorem in electromagnetic theory where the density of modes in a cavity is insensitive to the boundary of the system.

In this paper, perturbations and numerical errors are treated equally. Thus, a generalized error theory for the PDOS is formulated. Errors that occur when computing integrated quantities of the PDOS will not be considered because they have been discussed by Nex.[3]

In Sec. II, the recursion method for computing PDOS is discussed, and previous error analyses on the subject are briefly reviewed. It is seen that these analyses do not address the effects of numerical approximations like round-off errors on the PDOS. Hence in Sec. III, a generalization of the error theory for the PDOS is developed. This is used to examine the behavior of errors for systems where the PDOS has both discrete and continuous spec-

tra. This form of error theory for the recursion method takes into account all types of errors that occur in a recursion calculation. It extends the previous analysis given by Paige's theorem,[4-6] and the truncation effect discussed in Haydock[2] and Shohat and Tamarkin.[7] Examples of these errors include perturbations, round off, truncation of the recursion calculation, loss of orthogonality of the recursion vectors, and approximation in the Hamiltonian or non-Hermiticity. From this analysis, the accuracy of the computed PDOS is determined. To illustrate the insensitivity of the PDOS, a numerical example is discussed in Sec. IV. Section V summarizes the important features of the error theory and its application to the computational method known as dynamic recursion.[8]

II. THE RECURSION METHOD FOR COMPUTING PDOS

Given a Hamiltonian H and a starting orbital u_0, the recursion method is defined by the recurrence relation

$$Hu_0=a_0u_0+b_1u_1 \tag{4}$$

and for $n\geq 1$, by the three-term recurrence

$$Hu_n=a_nu_n+b_{n+1}u_{n+1}+b_nu_{n-1}\ . \tag{5}$$

From the a's and b's generated by the recurrence relation, the projected resolvent $R_0(E)$, in continued fraction form,[2] is

$$R_0(E)=\cfrac{1}{(E-a_0)-\cfrac{b_1^2}{(E-a_1)-\cfrac{b_2^2}{(E-a_2)-\cdots}}}\ . \tag{6}$$

The PDOS, $n(u_0;E)$, is proportional to the singular part of the projected resolvent. It is the limit as $\epsilon\rightarrow 0^+$, from above the real axis, of the imaginary part of $R_0(E)$:

$$n(u_0;E)=\lim_{\epsilon\rightarrow 0^+}-\frac{1}{\pi}\mathrm{Im}R_0(E+i\epsilon)\ . \tag{7}$$

In matrix notation, the recurrence relation is

$$HU=UJ\ , \tag{8}$$

where U is the matrix formed of the column vectors $u_0,u_1,u_2,\ldots,u_n$, and J is the symmetric tridiagonal matrix with the a_n's forming its diagonal elements and the b_n's its off-diagonal elements. By rewriting $HU=UJ$ into $U(E-J)^{-1}=(E-H)^{-1}U$, the projected resolvent is given by

$$\begin{aligned}R_0(E)&=(u_0,(E-H)^{-1}Ue_0)\\&=(u_0,U(E-J)^{-1}e_0)=\langle e_0,(E-J)^{-1}e_0\rangle\ ,\end{aligned} \tag{9}$$

where the parentheses denotes inner product in H space, the angled bracket denotes inner product in J space, u_0 is the starting orbital, e_k is the Cartesian basis vector in the J-space matrix representation, and the inner product $(u_i,u_j)=\delta_{ij}$.

Off the real axis, truncating the continued fraction after several steps gives a bounded error[2,7] on the projected resolvent which goes to zero as the number of recursion steps increases. Thus, it is not necessary to recur until the space is completely spanned in order to calculate the projected resolvent to a given precision. It can also be seen from the continued fraction how errors that occur further down its chain have a smaller effect on the projected resolvent.

Before proceeding with the generalized error analysis, a brief review of Paige's theorem and the analysis on truncation will be given in the following subsections.

A. Paige's theorem

Paige's theorem[4-6,9-13] can be briefly stated as follows: Let E be an eigenvalue of an $n\times n$ Hermitian matrix H with at most z nonzero elements in any row. If H is tridiagonalized using the recursion method, then after N recursion levels there exists an eigenvalue of the tridiagonal matrix J say μ_i, such that[12]

$$|E-\mu_i|\leq 2.5[|b_{N+1}u_i(N)|(1+2\epsilon_0)+2\epsilon_1\sqrt{N}\,\|H\|]\ , \tag{10}$$

where $\epsilon_0=(n+4)\epsilon$, $\epsilon_1=(7+z\alpha)\epsilon$, $\alpha\|H\|=\|\,|H|\,\|$ with $|H|$ the matrix formed by taking the absolute value of each element of H, ϵ the floating point error, b_{N+1} is the $N+1$ off-diagonal element of J, $u_i(N)$ is the Nth element of the ith recursion vector, and $\|H\|$ denotes the norm of the matrix H.

From the above relation, it is seen that Paige's theorem does not quantify how errors in the computed eigenvalues contribute to the computed projected resolvent. The eigenvalue μ_i is very sensitive to a change in the number of recursion levels while the projected resolvent is not. Furthermore, for an infinite system, the eigenvalue spectra is not necessary and so the result of Paige's theorem, while deals only with discrete eigenvalues, is inapplicable.

B. The effects of truncation

If the continued fraction is truncated after N levels, an error in the projected resolvent is introduced and the approximate projected resolvent[2,7] is given as a fractional linear transformation

$$R_0^N(E,z)=\frac{1}{b_1}\left[\frac{Q_{N+1}(E)-z\dfrac{Q_N(E)}{b_{N+1}}}{P_{N+1}(E)-z\dfrac{P_N(E)}{b_{N+1}}}\right]\ , \tag{11}$$

where z denotes the part of the continued fraction that has been truncated, $P_N(E)$ is an Nth order polynomial in E, and $Q_N(E)$ is an $(N-1)$th order polynomial. The polynomials satisfy the following relations:

$$\begin{aligned}&b_{n+1}P_{n+1}(E)=(E-a_n)P_n(E)-b_nP_{n-1}(E)\ ,\\&P_{-1}(E)=0\ \text{ and }\ P_0(E)=1\end{aligned} \tag{12}$$

$$\begin{aligned}&b_{n+1}Q_{n+1}(E)=(E-a_n)Q_n(E)-b_nQ_{n-1}(E)\ ,\\&Q_0(E)=0\ \text{ and }\ Q_1(E)=1\end{aligned} \tag{13}$$

and where the a's and the b's are the ones generated by Eq. (5).

Haydock[2] and Shohat and Tamarkin[7] have shown that for complex E and z, and for $N>0$, Eq. (11) maps the complex z plane into the interior of a circle $C(E)$ with the real axis of z mapping into the circumference of this circle. As N approaches infinity, the radius of this circle decreases monotonically to zero. From this result, it is seen that the recursion method gives a monotonically convergent sequence of approximations for the projected resolvent. However, this approach assumes an exact computation of the coefficients a_n and b_n. It does not address the effect of round-off errors that are encountered in practical applications. Nor does it determine the error on the PDOS when H is approximated.

III. GENERALIZED ERROR THEORY FOR THE RECURSION METHOD

In practical calculations, Paige's theorem cannot be applied in conjunction with the analysis on truncation because Paige's result does not apply to the projected resolvent. Hence the need for an error theory of the projected resolvent which does not assume exact arithmetic operations and which addresses the effects of other types of errors.

In this section, a generalized recurrence relation is given which includes an error term. This error term serves as the inhomogeneous part to the otherwise homogeneous matrix equation $HU=UJ$. The contribution of this inhomogeneous term to the projected resolvent for systems with extended or localized states is then analyzed.

A. The recursion method with an explicit error term

Consider the three-term recurrence relation of the recursion method as given by Eq. (5), and assume an error in each step of the recursion, represented by δ_n, such that the recurrence equation becomes

$$Hu_n=a_nu_n+b_{n+1}u_{n+1}+b_nu_{n-1}+\delta_n\ . \tag{14}$$

The term δ_n represents the most general type of error. Examples are perturbations, round off, truncation of the recursion process, loss of orthogonality of the recursion vectors, and approximation in the Hamiltonian or non-Hermiticity.

Consistent with the notations used in Sec. II, the equation above can be written in matrix form as

$$HU=UJ+\Delta\ , \tag{15}$$

where Δ is formed by the column vectors $\delta_0,\delta_1,\delta_2,\delta_3,\ldots,\delta_n$. When Δ is zero, the homogeneous matrix equation $HU=UJ$ is recovered. Equation (15) isolates the contribution of the error term from the a's and b's in the tridiagonal matrix J, and from the recursion vectors that forms U. Rewriting Eq. (15) to give an exact relation between the resolvent of H and the resolvent of J gives

$$R(E)U=UG(E)+R(E)\Delta G(E)\ , \tag{16}$$

where $R(E)=(E-H)^{-1}$ and $G(E)=(E-J)^{-1}$.

B. Error term in the projected resolvent

The projected resolvent for the starting orbital u_0 is the element in the first row and first column of Eq. (16), i.e.,

$$R_0(E)=G_0(E)+(u_0,R(E)\Delta G(E)e_0)\ , \tag{17}$$

where $R_0(E)=(u_0,(E-H)^{-1}u_0)$, $G_0(E)=\langle e_0,(E-J)^{-1}e_0\rangle$, and u_0 and e_0 were defined in Sec. II. In this form, the error on the projected resolvent $R_0(E)$ is entirely contained in $(u_0,R(E)\Delta G(E)e_0)$.

Now consider the behavior of $(u_0,R(E)\Delta G(E)e_0)$. First expand it in the basis, $\{\Phi_n\}$, of the Hamiltonian H and also in the basis $\{e_k\}$ of the tridiagonal matrix J which were defined in Sec. II. Without loss of generality, Φ_0 is chosen as the starting orbital. Then the error term of the projected resolvent is given by

$$(\Phi_0,R(E)\Delta G(E)e_0)=\sum_{n,k}(\Phi_0,(E-H)^{-1}\Phi_n)\times(\Phi_n,\Delta e_k)\langle e_k,(E-J)^{-1}e_0\rangle\ . \tag{18}$$

Note that $(\Phi_n,\Delta e_k)$ is the n by k element of the matrix Δ. The other two terms in the product are off-diagonal elements of the exact and computed resolvent, i.e., $R_{0n}(E)=(\Phi_0,(E-H)^{-1}\Phi_n)$ and $G_{k0}(E)=\langle e_k,(E-J)^{-1}e_0\rangle$, respectively. The error in the projected resolvent is determined by how Δ couples to the off-diagonal elements of the resolvent;

$$(\Phi_0,R(E)\Delta G(E)e_0)=\sum_{n,k}R_{0n}(E)\Delta_{nk}G_{k0}(E)\ . \tag{19}$$

C. Behavior of the off-diagonal element of the resolvent

Next the behavior of $(\Phi_0,R(E)\Delta G(E)e_0)$ for systems that have either an exponentially localized or extended states will be considered. Cases in between should be clear from these two extremes. The expression for $R_{0n}(E)$ and $G_{k0}(E)$ have to be generalized for systems with extended states. Since $R_{0n}(E)$ and $G_{k0}(E)$ have similar form, only $R_{0n}(E)$ will be considered; results for $R_{0n}(E)$ are also valid for $G_{k0}(E)$.

In a system with extended states, $R_{0n}(E)$ is given by an integral over an energy distribution. The off-diagonal element of the resolvent becomes

$$R_{0n}(E)=(\Phi_0,(E-H)^{-1}\Phi_n)\equiv\int_{-\infty}^{\infty}\frac{(\Phi_0,\Psi(E'))(\Psi(E'),\Phi_n)}{(E-E')}n(\Phi_0;E')dE'\ , \tag{20}$$

where $(\Psi(E'),\Phi_n)$ is the inner product of the orbital Φ_n and the state $\Psi(E')$. It is the projection of the orbital Φ_n onto the eigenstate Ψ with an energy E'. Here, the PDOS, $n(\Phi_0,E)$, is chosen as the energy distribution function. This choice of energy distribution function $n(\Phi_0,E)$ defines the normalization condition for the wave function Ψ. [The relation between the choice of energy

distribution function $n(\Phi_0,E)$ and the normalization condition of the wave function Ψ is discussed in the Appendix.]

1. Localized eigenstates

Exponentially localized eigenstates give rise to singular spectral points (δ-function distribution of states) in the PDOS. Since the eigenstate Ψ_α is exponentially localized, its overlap with the orbital Φ_n decreases exponentially with distance x_n from the center of Ψ_α which is taken to be the origin, i.e.,

$$(\Psi(E_\alpha),\Phi_n)\sim e^{-k_\alpha x_n} . \tag{21}$$

For large n and E near E_α, from Eq. (20), the off-diagonal elements of the resolvent, $R_{0n}(E)$, goes to zero exponentially with x_n:

$$R_{0n}(E)\sim\frac{e^{-k_\alpha(x_0+x_n)}}{E-E_\alpha} . \tag{22}$$

2. Extended states

With extended states, the PDOS is a smooth (absolutely continuous) spectrum. Here, the states are assumed to have a free-particle-like behavior which gives

$$(\Psi(E'),\Phi_n)\sim e^{i\theta_n(E')} , \tag{23}$$

where $\theta_n(E')$ varies smoothly as a function of E'. The function $e^{i\theta_n(E')}$ is a generalization of the free-particle expression $e^{ik(E')x_n}$.

Since $n(\Phi_0,E')$ is smooth, substituting this and Eq. (23) into Eq. (20) gives

$$\mathrm{Re}R_{0n}(E)\sim n(\Phi_0;E)\sin[\theta_n(E)]e^{-\epsilon\theta_n'(E)} , \tag{24}$$

and

$$-\frac{1}{\pi}\mathrm{Im}R_{0n}(E)\sim n(\Phi_0;E)\cos[\theta_n(E)]e^{-\epsilon\theta_n'(E)} , \tag{25}$$

where, when integrating Eq. (20), $n(\Phi_0,E')$ is evaluated at E and $\theta_n(E')$ has been expanded around E as $\theta_n(E')\sim\theta_n(E)+\theta_n'(E)(E'-E)$. In order to make the integral nonsingular, the projected resolvent is evaluated for complex $E\to E+i\epsilon$. These off-diagonal elements of the resolvent dies off exponentially fast when $\theta_n'(E)\gg 1/\epsilon$.

The contribution of Eq. (19) to integrated quantities of the projected resolvent is thus proportional to

$$\int f(E)e^{-\epsilon\theta'(E)}\cos[\theta_n(E)]dE . \tag{26}$$

This goes to zero exponentially fast for $\epsilon\neq 0$. On the real axis when $\epsilon=0$, this integral is the Fourier transform of $f(E)$ and also goes to zero exponentially in the limit as $\theta_n(E)\to\infty$ provided that $f(E)$ is smooth and $\int_{-\infty}^{\infty}|f(E)|dE<\infty$.

D. Relation to previous error theories

One can recover the results given in Haydock[2] and Shohat and Tamarkin[7] when the continued fraction is truncated. Equation (11) in Sec. II B gives the expression for $R_0^N(E,z)$. $G_0(E)$ follows from Eq. (11) when $z=0$, that is, if the continued fraction has terminated. So $(\Phi_0,R(E)\Delta G(E)e_0)$ is given by

$$R_0(E)-G_0(E)=\frac{b_{N+1}Q_{N+1}(E)-zQ_N(E)}{b_1[b_{N+1}P_{N+1}(E)-zP_N(E)]}-\frac{Q_{N+1}(E)}{b_1P_{N+1}(E)} . \tag{27}$$

Simplifying the equation gives the form of the error in the projected resolvent, $(\Phi_0,R(E)\Delta G(E)e_0)$, in terms of the truncation error of the continued fraction z as

$$(\Phi_0,R(E)\Delta G(E)e_0)=\frac{z[Q_{N+1}(E)P_N(E)-P_{N+1}(E)Q_N(E)]}{b_1P_{N+1}(E)[b_{N+1}P_{N+1}(E)-zP_N(E)]} . \tag{28}$$

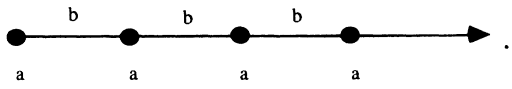
This is a linear fractional transformation which has the same property mentioned in Sec. II B and discussed in Haydock or Shohat and Tamarkin.

Paige's theorem results directly from Eq. (15). Hence the relation $HU=UJ+\Delta$ serves as a starting point for deriving Paige's theorem. These are shown in Refs. 9 and 10.

It is seen that Paige's theorem has been incorporated into an error theory for the projected resolvent which also takes into account the effects of truncation and other types of error. Thus all forms of error that accrue during the recursion process have been considered in this generalized error theory for the projected resolvent.

IV. NUMERICAL EXAMPLE

A simple nontrivial example is the π-bonded linear chain. It is a series of atomic orbitals concatenated to form a chain. The Hamiltonian is composed of the on-site energy a of each orbital and a hopping interaction b which is between its nearest neighbors.



Taking the starting state u_0 to be the left-most orbital, this model give the a's and b's in the tridiagonal matrix as[2]

$$a_n=a,\quad b_n=b . \tag{29}$$

Whence, this system is also known as the constant chain model. This model gives a discrete or continuous spectra depending on whether the chain is finite or infinite, respectively. For an infinitely long chain, the analytic expression for the PDOS of the orbital at the left-most site is

$$n(u_0;E)=\begin{cases}\sqrt{4b^2-(E-a)^2}/4b^2, & a-2b\le E\le a+2b ,\\ 0, & E<a-2b, E>a+2b .\end{cases} \tag{30}$$

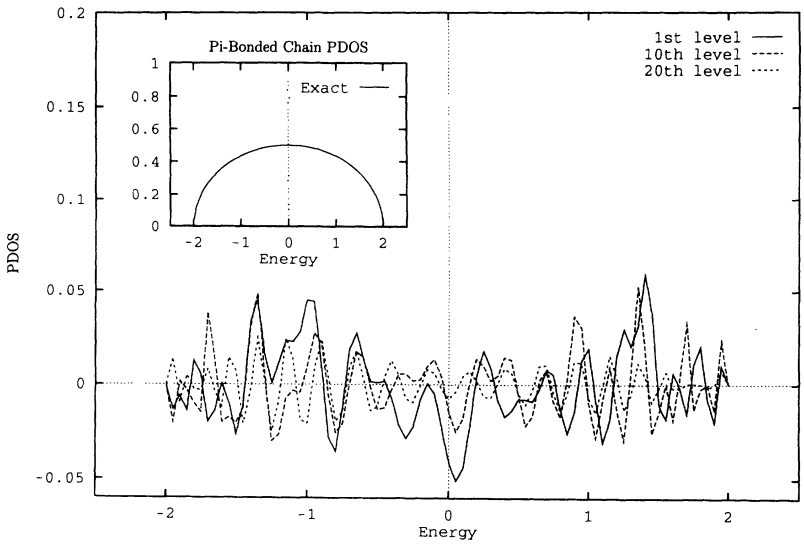


FIG. 1. A plot of the differences between the exact PDOS and those with rounding errors that occur at different recursion levels. The solid curve is when errors begin at level $n \geq 1$. The dashed curve is when errors start from $n \geq 10$ while the dotted curve is when $n \geq 20$. All calculations were terminated using the square-root terminator after 25 recursion levels. Inset is a plot of the exact PDOS as given by the analytic expression of Eq. (30). The values used for a and b are $a=0$, $b=1$.

To see how the PDOS is affected by perturbations, errors are introduced into the numerical calculation at different recursion levels, i.e., for $n \geq 1$, 10, and 20; corresponding to different proximity of the perturbation from the starting orbital. All calculations were terminated after 25 recursion levels with the same square-root terminator.[2,3,14] Without loss of generality, the following values were used for a and b: $a=0$ and $b=1$. Errors introduced are such that $|\delta_n| \leq 0.01$ in Eq. (14); which is less than 10% of u_n. The term δ_n manifests itself as errors on the tridiagonal coefficients a_n and b_n. The differences between the exact PDOS and the perturbed ones are plotted in Fig. 1. A plot of the exact PDOS is provided (inset) for reference. It is seen that errors that occur early in the recursion make a bigger change on the PDOS. This is consistent with the fact that perturbations nearby has a much larger effect on the local environment. As errors occur later in the recursion process, which is equivalent to perturbations farther from the starting state, the changes in the PDOS get smaller. Note that the maximum deviation in the PDOS is also less than 10% of its exact value. Moreover, note how the changes in the PDOS oscillates between positive and negative values which then cancels out when calculating integrated quantities like $\langle n \rangle$ or $\langle E \rangle$ of Eqs. (2) and (3), respectively. Also it can be seen from Fig. 1 that the band edges have converged as expected with a recursion calculation. From this plot, one clearly sees the insensitivity of the PDOS to errors which are far from the starting state u_0. This is an example of the black-body character of the PDOS.

V. BLACK-BODY THEOREM AND DYNAMIC RECURSION

A. Summary

The general form of error on the resolvent is given by Eqs. (16) and (17). The error term in these equations includes the effect of truncation and Paige's theorem. Furthermore, it is seen that for localized systems the error term $(u_0, R(E)\Delta G(E)e_0)$ decays exponentially with distance from the starting orbital. The computed resolvent $G_0(E)$ converges exponentially with decreasing error to its exact value $R_0(E)$. For systems with extended states, it was shown that the contribution of $(u_0, R(E)\Delta G(E)e_0)$ to $R_0(E)$ is zero in the mean.

B. Application

The error in the projected resolvent given by Eq. (19), which dies off exponentially as a function of distance from the starting orbital, describes the insensitivity of the PDOS to disturbances far from the orbital in consideration, or to the system's boundary conditions. This insensitivity is a form of a black-body theorem for the projected density of states. This is the basis for dynamic recursion.[8]

Dynamic recursion makes use of this black-body effect of the PDOS to implement a computational method that uses a dynamic basis set to handle an infinite system. In this scheme, only the N largest elements of the recursion vector are considered. The neglected components are then treated as errors in the recursion process with the largest of these neglected components serving as an upper bound for the error δ in $HU = UJ + \Delta$. Although Paige's theorem is inapplicable because there need not be discrete eigenvalues for an infinite system, projected quantities like PDOS can still be calculated and their errors bounded. Using the analysis given in Sec. III, the error on the projected resolvent, $(u_0, R(E)\Delta G(E)e_0)$, and its integrated quantities can be determined. The generalized error analysis for the projected resolvent shows that the computed projected quantities have bounded errors and that the projected resolvent converges monotonically to its exact value as the approximation improved. This result allows the use of a dynamic basis set in a recursion calculation for an infinite system.

ACKNOWLEDGMENTS

We would like to acknowledge the Condensed Matter Theory group at the University of Oregon for stimulating and useful discussions, specifically to A. Gibson and P.

Bunson. Similarly, we would like to thank W. M. C. Foukes and J. F. Annett for encouraging and helpful discussion. This work was supported in part by the National Science Foundation under Grant No. DMR-9319246.

APPENDIX: OFF-DIAGONAL ELEMENTS OF THE RESOLVENT AND NORMALIZATION CONDITION

For a general expression of the projected resolvent which includes extended states, $R_{0n}(E)$ is given as an integral over an energy distribution; the total density of states. However, the choice for an energy distribution function is not limited to the total density of states. Any energy distribution from an invariant subspace that contains either Φ_0 or Φ_n is acceptable provided that the wave functions be normalized accordingly.

If the PDOS, $n(\Phi_0,E)$, is chosen as the energy distribution, that is,

$$R_{0n}(E)=(\Phi_0,(E-H)^{-1}\Phi_n) \equiv \int_{-\infty}^{\infty} \frac{(\Phi_0,\Psi(E'))(\Psi(E'),\Phi_n)}{(E-E')} n(\Phi_0;E')dE' , \tag{A1}$$

where $(\Psi(E'),\Phi_n)$ is the inner product of the orbital Φ_n and the wave function $\Psi(E')$, then $\Psi(E')$ has to be normalized in a way that $R_{0n}(E)=(\Phi_0,(E-H)^{-1}\Phi_n)$ becomes equal to the integral expression on the right-hand side of Eq. (A1).

Consider the case for which the PDOS is a distribution of localized states. The spectrum is singular and discrete, i.e., the PDOS is given by a set of δ-function such that

$$n(\Phi_0;E)=\sum_\alpha w_\alpha \delta(E-E_\alpha) , \tag{A2}$$

where w_α is the probability of the orbital Φ_0 to be on the state $\Psi(E_\alpha)$ with energy E_α.

Substituting this form of the PDOS into Eq. (A1), and integrating over all energy, the zero-zero element of the projected resolvent is given as

$$R_0(E)=R_{00}(E)=\sum_\alpha \frac{w_\alpha |(\Psi(E_\alpha),\Phi_0)|^2}{(E-E_\alpha)} . \tag{A3}$$

But $-(1/\pi)\mathrm{Im}R_0(E)$ is the PDOS, so from Eqs. (A2) and (A3), this makes $|(\Psi(E_\alpha),\Phi_0)|^2=1$. This type of normalization for the wave function $\Psi(E_\alpha)$ is associated with the choice of the PDOS for the energy distribution. This construction is known as point normalization. Hence the distribution function chosen in Eq. (A1) to define the off-diagonal element of the resolvent sets the normalization for the wave function $\Psi(E_\alpha)$.

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