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Simple approach to self-energy corrections in semiconductors and insulators

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We have used the Sterne-Inkson [P. A. Sterne and J. C. Inkson, J. Phys. C 17, 1497 (1984)] extreme tight-binding model for the self-energy corrections to the top of the valence band and bottom of the conduction band within the *GW* approximation. Application of these corrections to both exchange-only local-density-approximation (LDA) calculations and the LDA with Ceperley-Alder correlation calculations for five materials C, Si, Ge, GaAs, and ZnSe has been found to result in good agreement with experimental data and recent theoretical results. The LDA calculations were performed by using the plane-wave-basis and norm-conserving pseudopotentials.

I. INTRODUCTION

The *ab initio* calculation of quasiparticle energies in semiconductors and insulators has proven to be an intractable problem for several years. The powerful local-density approximation[1] (LDA) to density-functional theory[1,2] (DFT) has been shown to be inadequate in such situations despite its success in calculations on a wide range of metals. It was proved as early as 1971 by Kane[3] that a local potential would never be sufficient to describe the electronic properties of semiconductors and insulators, due to the nonuniform distribution of electrons in such materials. However, further work throughout the 1970s suggested an equally important difficulty due to the energy dependence of many-body effects,[4] which is ignored in DFT.

Neglect of these two effects leads to inaccurate predictions of both ground-state and excited-state properties within the LDA. In the case of the ground-state properties the problems are small (e.g., lattice constants are reproduced reasonably well but cohesive energies are systematically slightly overestimated[5]) but the calculated excited-state properties in semiconductors and insulators are very inaccurate with band gaps typically underestimated by 50% or more. The fault may be traced to the fact that the DFT is essentially a ground-state formalism, having its basis in variational arguments with the electron density of occupied states as the fundamental variable. Thus, although it could be expected to be accurate for valence-band states, its predictions for excited states (i.e., conduction bands) should not be considered to be physically relevant. However, in metals it seems that the predicted conduction bands do match experiment reasonably well whereas in semiconductors and insulators they do not.[6,7]

The surprise is not that the LDA does not work for semiconductors and insulators, but that it works so well in metals. The reason would appear to be that the density-functional formalism involves a single exchange-correlation potential for all bands, whereas it has been shown that in systems with a band gap the exchange-correlation potential ought to be discontinuous across the band gap.[6,7] In metals there is no problem because there is no band gap, but in insulators and semiconductors this discontinuity is missed entirely by DFT, no matter what improvements upon the LDA are made (e.g., gradient expansions or weighted density approximation[8]). The effect of this discontinuity is thought to be responsible for up to 80% of the error in the LDA band gaps, the other 20% being due to the local approximation itself.[9]

With this new understanding of the deficiencies in DFT and the advent in the early 1980s of reliable *ab initio* pseudopotential calculations[5] there was a renewed interest in the quantitative discussion of many-body effects in semiconductors.

The common alternative to the DFT "single-particle" approach is the self-energy "quasiparticle" approach based upon field-theory techniques, which had been investigated throughout the 1970s both in a qualitative sense and computationally in the context of empirical pseudopotential calculations.[4] The method accounts for the many-body interactions by the use of a nonlocal, energy-dependent "self-energy" operator, $\Sigma(\mathbf{r},\mathbf{r}';\omega)$. The self-energy is defined in full by a self-consistent set of equations, the Hedin equations,[10,11] which led to its expression as the sum of an infinite series. It is usual to take only the first term of the series, the *GW* approximation, which has the form

$$\Sigma(\mathbf{r},\mathbf{r}';\omega)=\frac{i}{2\pi}\int d\omega' G(\mathbf{r},\mathbf{r}';\omega-\omega')W(\mathbf{r},\mathbf{r}';\omega')e^{i\delta\omega'} , \tag{1.1}$$

where $G(\mathbf{r},\mathbf{r}';\omega)$ is the many-body Green's function, $W(\mathbf{r},\mathbf{r}';\omega)$ is the screened electron-electron interaction, and δ is an infinitesimally small positive quantity. An accurate evaluation of the self-energy is the key to the band-structure problem. Self-consistent solutions of the Kohn-Sham equations[1] using the LDA and *ab initio* pseudopotentials provide a reliable basis set to allow quantitative determination of the energy-dependent and nonlocal properties of the self-energy. Thus a detailed discussion of many-body effects in solids is at last possible. A word of caution is in order. Although it is believed that the self-energy series is sufficiently well converged that the first term is dominant and further terms need not be con-

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sidered, and despite the widespread use of this approximation over several years, little quantitative work has been undertaken to confirm that it is indeed justified.[12]

Once the matrix elements of $\Sigma(\mathbf{r},\mathbf{r}';\omega)$ are calculated they can be used to give corrections to the energy eigenvalues calculated in any other simpler scheme (usually the LDA). The major difficulty lies in the evaluation of these matrix elements due to the nonlocal and energy-dependent nature of the self-energy operator. Several methods of calculation, of varying degrees of complexity, have been discussed in the literature, and indeed are the subject of current debate. What is clear is that full self-energy calculations are extremely computationally demanding and this restricts the application of this formalism to only the simplest cases. There is, therefore, much interest in simplified versions of the *GW* approximation, which may allow more physically interesting problems to be tackled. One particularly simple approach is the extreme tight-binding method proposed by Sterne and Inkson.[13] In this paper we present an extended version of the Sterne-Inkson method which corrects an error in the earlier paper[13,14] and includes a more complete discussion of the on-site exchange term $\mathcal{C}$ in the light of comments in the literature.[15] Details are given in Sec. III and the results of our calculations using this model for the materials C, Si, Ge, GaAs, and ZnSe are presented in Sec. IV. In Sec. V we compare our results with those of other workers who have used alternative *GW*-based techniques.

II. REVIEW OF THE STERNE-INKSON MODEL

In order to evaluate $\Sigma(\mathbf{r},\mathbf{r}';\omega)$ in the case of semiconductors and insulators Sterne and Inkson[13,14] used an extreme tight-binding (ETB) basis set and a two-band model with constant band gap E_g. Accordingly we write for diamond and zinc-blende structures

$$\psi_{\mathbf{k}\nu}^n(\mathbf{r})=\left[\frac{2}{N}\right]^{1/2}\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\phi_\nu^n(\mathbf{r}-\mathbf{R}) , \tag{2.1}$$

where ν is a bond index (four bonds per atom for tetrahedral coordination), n is a band index (either v or c for valence or conduction band), $\mathbf{R}$ is a cell index, N is the number of fcc cells, and ϕ_ν^n is a Wannier function obeying the orthonormality relation

$$\int d^3r\, \phi_\nu(\mathbf{r}-\mathbf{R})\phi_{\nu'}(\mathbf{r}-\mathbf{R}')=\delta_{\nu\nu'}\delta_{\mathbf{R}\mathbf{R}'} . \tag{2.2}$$

The Green's function $G(\mathbf{r},\mathbf{r}';\omega)$ may then simply be written in the standard biorthonormal form[16] as

$$G(\mathbf{r},\mathbf{r}';\omega)=\sum_{n,\nu,\mathbf{R}}\frac{\phi_\nu^n(\mathbf{r}-\mathbf{R})\phi_\nu^{n*}(\mathbf{r}'-\mathbf{R})}{\omega-E_n\pm i\delta} . \tag{2.3}$$

In contrast to $G(\mathbf{r},\mathbf{r}';\omega)$ the evaluation of $W(\mathbf{r},\mathbf{r}';\omega)$ requires careful consideration. It is usually approximated by some form of generalized-plasmon-pole (GPP) approximation[17] or more recently it has been represented in a biorthonormal form analogous to that of the Green's function.[18,19] The approach of Sterne and Inkson was to simply take the standard random-phase-approximation[11,20] form of the dielectric function within the two-band ETB model

$$\varepsilon(\mathbf{r},\mathbf{r}';\omega)=\delta(\mathbf{r}-\mathbf{r}')-N_0(\omega)\sum_{\mathbf{R},\nu}\int d^3r''v(\mathbf{r}-\mathbf{r}'')A_\nu(\mathbf{r}''-\mathbf{R})A_\nu^*(\mathbf{r}'-\mathbf{R}) , \tag{2.4}$$

where $N_0(\omega)=-4E_g/(E_g^2-\omega^2)$, $A_\nu(\mathbf{r}-\mathbf{R})=\phi_\nu^{c*}(\mathbf{r}-\mathbf{R})\phi_\nu^v(\mathbf{r}-\mathbf{R})$, and $v(\mathbf{r}-\mathbf{r}')$ is the bare electron-electron interaction. This simple approach to ε allows its inversion in real space[21,22] to give

$$\varepsilon^{-1}(\mathbf{r},\mathbf{r}';\omega)=\delta(\mathbf{r}-\mathbf{r}')-\frac{4E_g}{E_g^2+(\hbar\omega_p)^2-\omega^2}\sum_{\mathbf{R},\nu}\int d^3r''v(\mathbf{r}-\mathbf{r}'')A_\nu(\mathbf{r}''-\mathbf{R})A_\nu^*(\mathbf{r}'-\mathbf{R}) , \tag{2.5}$$

with $\hbar\omega_p$ representing the plasmon energy.

The screened interaction may then be simply found since

$$W(\mathbf{r},\mathbf{r}';\omega)=\int d^3r''\varepsilon^{-1}(\mathbf{r},\mathbf{r}'';\omega)v(\mathbf{r}''-\mathbf{r}') , \tag{2.6}$$

which together with (2.5) finally yields

$$W(\mathbf{r},\mathbf{r}';\omega)=v(\mathbf{r}-\mathbf{r}')-\frac{4E_g}{E_g^2+(\hbar\omega_p)^2-\omega^2}\times\sum_{\mathbf{R},\nu}D_\nu(r-\mathbf{R})D_\nu^*(\mathbf{r}'-\mathbf{R}) , \tag{2.7}$$

in which $D_\nu(\mathbf{r}-\mathbf{R})=\int d^3r'\,A_\nu(\mathbf{r}'-\mathbf{R})v(\mathbf{r}-\mathbf{r}')$ represents the dipole moment at $\mathbf{r}$ due to bond ν in cell $\mathbf{R}$.

It can be noted that this analytical expression retains the most important properties of the screened interaction, namely, poles at the plasmon energies and a zero near the band-gap energy. In addition, it is presented in real space and so application of this approach to surfaces and interfaces is reasonably straightforward. Indeed, analytic limits based on the Sterne-Inkson formalism have already been used to discuss the band-gap changes near heterojunction interfaces[23] and work is in progress to apply the method outlined in the present paper to these situations. The results of such calculations will be presented in a future publication.

From (1.1) it can be seen that the self-energy is composed of two contributions: one due to the poles in the Green's function and the other due to the poles in the screened interaction. Since the poles of $W(\mathbf{r},\mathbf{r}';\omega)$ represent the plasmon energies, it is natural to regard this contribution as being due to the cloud of virtual plasmons which constantly surrounds the quasielectron. In a classical sense this may be regarded as the Coulomb hole contribution (CHC). We may regard the other contribution as being due to screened exchange (SX) and so write

$$\Sigma(\mathbf{r},\mathbf{r}';\omega)=\Sigma_{\mathrm{SX}}(\mathbf{r},\mathbf{r}';\omega)+\Sigma_{\mathrm{CHC}}(\mathbf{r},\mathbf{r}';\omega) \ . \tag{2.8}$$

In principle, the eigenvalues of the system are then found by solving

$$[H_0(\mathbf{r})+V_H(\mathbf{r})]\psi^n(\mathbf{r})+\int d^3r'\Sigma(\mathbf{r},\mathbf{r}';E_n)\psi^n(\mathbf{r}') =E_n\psi^n(\mathbf{r}) \ , \tag{2.9}$$

where H_0 is the noninteracting Hamiltonian and V_H is the Hartree potential. Sterne and Inkson suggested replacing the troublesome nonlocal potential $\Sigma(\mathbf{r},\mathbf{r}';\omega=E_n)$ with the simple local but band-dependent potential

$$\int d^3r'\Sigma(\mathbf{r},\mathbf{r}';\omega=E_n)\psi^n_{k,\nu}(\mathbf{r}')=V^n_{\mathrm{xc}}(\mathbf{r})\psi^n_{k,\nu}(\mathbf{r}) \ . \tag{2.10}$$

After some algebra[13,14] the local potentials can be expressed as

$$V^v_{\mathrm{SX-CHC}}(\mathbf{r})=-e^2\rho^{1/3}(\mathbf{r})\frac{\gamma}{2}\left[\frac{2\pi}{3}\right]^{1/3}\left[1+\frac{1}{\varepsilon_0}\right] -\frac{\mathcal{C}}{2}\left[\frac{\varepsilon_0-1}{\varepsilon_0+\sqrt{\varepsilon_0}}\right] , \tag{2.11}$$

$$V^c_{\mathrm{SX-CHC}}(\mathbf{r})=-e^2\rho^{1/3}(\mathbf{r})\frac{\gamma}{2}\left[\frac{2\pi}{3}\right]^{1/3}\left[1-\frac{1}{\varepsilon_0}\right] -\frac{\mathcal{C}}{2}\left[\frac{\varepsilon_0-1}{\varepsilon_0-\sqrt{\varepsilon_0}}\right] , \tag{2.12}$$

where

$$\mathcal{C}=\int d^3r\, d^3r'\, A^*_\nu(\mathbf{r}-\mathbf{R})v(\mathbf{r}-\mathbf{r}')A_\nu(\mathbf{r}'-\mathbf{R}) \tag{2.13}$$

is an on-site exchange interaction and the sum-rule-derived relation

$$\varepsilon_0\cong\frac{E_g^2+(\hbar\omega_p)^2}{E_g^2} \tag{2.14}$$

has been introduced to relate the model energy gap to the known dielectric constant of the semiconductor. The constant γ arises as the result of an angular average over the bonds at a site. Noting the similarity of (2.11) and (2.12) to the LDA exchange-only potential[1]

$$V_X^{\mathrm{LDA}}(\mathbf{r})=-e^2\left[\frac{3}{\pi}\right]^{1/3}\rho^{1/3}(\mathbf{r}) \ , \tag{2.15}$$

it is natural to choose γ such that both the Sterne-Inkson potentials tend to the LDA potential in the limit as $\varepsilon_0\rightarrow\infty$ (i.e., increasing metallicity) since in this limit the LDA potential is expected to be accurate. The value of γ thus obtained is

$$\gamma=2\left[\frac{9}{2\pi^2}\right]^{1/3} , \tag{2.16}$$

which is, in any case, close to the angular average. It is important to note that although these potentials do bear a striking resemblance to the LDA form, they have been derived entirely within a formalism that recognizes from the start the localized nature of the electronic distribution in semiconductors and insulators, a situation quite unlike that for which the LDA is derived. This may be taken as further evidence that it is primarily the DFT that is to blame for the failure of the LDA in such cases rather than the failure of the local-density-based potential.

The exchange parameter $\mathcal{C}$, defined in (2.13), is significant. Sterne and Inkson[13,14] used the value 2.6 eV in the case of diamond and scaled this result inversely with the lattice constant to find estimates for other group-IV semiconductors, because of the similarity in the shape of the bond orbitals of these materials.[14,24,25] It is worth considering the physical origin of $\mathcal{C}$ in more detail, however. We denote the sp^3 hybrid atomic orbitals from a pair of atoms A and B by ξ_a and ξ_b. The bonding and antibonding Wannier orbitals of the solid can be written as

$$\phi^v=\frac{(\xi_a+f_c\xi_b)}{(1+f_c^2)^{1/2}} , \tag{2.17}$$

$$\phi^c=\frac{(f_c\xi_a-\xi_b)}{(1+f_c^2)^{1/2}} , \tag{2.18}$$

where the f_c is the fraction of covalent character, or unity minus the fraction of ionic character f_i.[26] In terms of these hybrid atomic orbitals, we can write $\mathcal{C}$ as

$$\mathcal{C}=\frac{1}{(1+f_c^2)^2}\int\left\{\xi_a\xi_b\frac{1}{|\mathbf{r}-\mathbf{r}'|}\xi_a\xi_b +f_c^2\left[(\xi_a^2-\xi_b^2)\frac{1}{|\mathbf{r}-\mathbf{r}'|}(\xi_a^2-\xi_b^2) -2\xi_b\xi_a\frac{1}{|\mathbf{r}-\mathbf{r}'|}\xi_a\xi_b\right] +f_c^4\xi_b\xi_a\frac{1}{|\mathbf{r}-\mathbf{r}'|}\xi_b\xi_a\right\}d^3r\, d^3r' , \tag{2.19}$$

where, in each term, the first pair of orbitals corresponds to the electron situated at $\mathbf{r}$ and the second pair corresponds to the electron at $\mathbf{r}'$. We have calculated the basic integrals in the case of diamond by using Slater atomic orbitals[27,28] with an effective nuclear charge of 3.5.[29] The values of the integrals are as follows:

TABLE I. Parameters used in the present work.

	a (Å)	ε_0	$\mathcal{C}$ (eV)
Diamond	3.55	5.7	3.94
Si	5.43	11.9	1.67
Ge	5.66	16.0	1.56
GaAs	5.65	10.9	1.61
ZnSe	5.66	5.9	1.86

$$\begin{aligned}&\int \xi_a^2 \frac{1}{|\mathbf{r}-\mathbf{r}'|}\xi_a^2 d^3r\, d^3r' = 18.63 \text{ eV} ,\\ &\int \xi_a^2 \frac{1}{|\mathbf{r}-\mathbf{r}'|}\xi_b^2 d^3r\, d^3r' = 10.76 \text{ eV}, \qquad (2.20)\\ &\int \xi_a \xi_b \frac{1}{|\mathbf{r}-\mathbf{r}'|}\xi_a \xi_b d^3r\, d^3r' = 5.12 \text{ eV} .\end{aligned}$$

Making the usual approximation that tight-binding matrix elements scale inversely with the square of the lattice constant irrespective of ionicity,[30] it is simple to estimate the values of the basic integrals in other materials based upon these calculations. Taking values of f_i from Ref. 26 we have calculated $\mathcal{C}$ for five materials, obtaining the values listed in Table I.

This approach has a much firmer physical basis than the simple approach taken by Sterne and Inkson. It is clear that a full calculation of $\mathcal{C}$ would be much more preferable to this estimation scheme, but in the context of the approximations already made, the method we have proposed seems to be quite adequate to enable reliable calculations to be made.

III. DETAILS OF THE CALCULATION

Our approach lies in using the Sterne-Inkson potentials to evaluate the corrections to the eigenvalues produced within the LDA. For calculating LDA eigensolutions we use the plane-wave basis and *ab initio*, norm-conserving pseudopotentials.[31] Plane waves up to the kinetic-energy cutoff of 14 Ry were considered for all the materials except diamond, for which a 50-Ry cutoff was required for well-converged results. No relativistic effects (e.g., spin-orbit interaction) were included. LDA results were obtained for both pure exchange (referred to as LDA/EX further in the paper) and exchange plus Ceperley-Alder correlation[32] (referred to as LDA/CA).

The calculation of the self-energy corrections to the eigensolutions should involve a first-order estimate based on the LDA results, followed by an iterative procedure to achieve a self-consistent solution. However, the work of Hybertsen and Louie[17] shows that if this approach is followed the eigenfunctions found after the first iteration overlap 99.9% with the LDA eigenfunctions. The implication is that although the LDA eigenvalues are incorrect, the LDA eigenfunctions are, for all practical purposes, identical to the true eigenfunctions of the system. Thus, since the matrix elements of $V_{\text{xc}}^{v}(\mathbf{r})$ and $V_{\text{xc}}^{c}(\mathbf{r})$ depend only on the eigenfunctions and the electron density (itself a functional of the eigenfunctions) we may safely say that our first-order estimate of the eigenvalues is accurate and that no further iterations are necessary. The corrections to the LDA eigenvalues are then given by

$$\Delta E_{\mathbf{k}}^{v} = \langle \psi_{\mathbf{k}}^{v}(\mathbf{r}) | V_{\text{xc}}^{v}(\mathbf{r}) | \psi_{\mathbf{k}}^{v}(\mathbf{r}) \rangle - \langle \psi_{\mathbf{k}}^{v}(\mathbf{r}) | V_{\text{xc}}^{\text{LDA}}(\mathbf{r}) | \psi_{\mathbf{k}}^{v}(\mathbf{r}) \rangle , \qquad (3.1)$$

$$\Delta E_{\mathbf{k}}^{c} = \langle \psi_{\mathbf{k}}^{c}(\mathbf{r}) | V_{\text{xc}}^{c}(\mathbf{r}) | \psi_{\mathbf{k}}^{c}(\mathbf{r}) \rangle - \langle \psi_{\mathbf{k}}^{c}(\mathbf{r}) | V_{\text{xc}}^{\text{LDA}}(\mathbf{r}) | \psi_{\mathbf{k}}^{c}(\mathbf{r}) \rangle . \qquad (3.2)$$

In a plane-wave expansion we express

$$\psi_{\mathbf{k}}^{n}(\mathbf{r}) = \frac{1}{\sqrt{N_0 \Omega}} \sum_{\mathbf{G}} A_{n\mathbf{k}}(\mathbf{G}) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} , \qquad (3.3)$$

where n is a band index, N_0 is the number of unit cells, Ω is the volume of a unit cell, and the potentials $V_{\text{xc}}^{v,c}$ and $V_{\text{xc}}^{\text{LDA}}$ may be written in a Fourier expanded form so that

$$V_{\text{xc}}(\mathbf{r}) = \sum_{\mathbf{G}} V_{\text{xc}}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}} . \qquad (3.4)$$

Substituting the exchange-only LDA potential from (2.15) and the Sterne-Inkson potentials given in (2.11) and (2.12), we find that we must evaluate

$$\Delta E_{\mathbf{k}}^{v} = -e^2 \left[\frac{3}{\pi} \right]^{1/3} \frac{1}{\varepsilon_0} \times \sum_{\mathbf{G},\mathbf{G}'} A_{n\mathbf{k}}^{*}(G') A_{n\mathbf{k}}(\mathbf{G}) \rho^{1/3}(\mathbf{G}'-\mathbf{G}) - \frac{\mathcal{C}}{2} \left[\frac{\varepsilon_0 - 1}{\varepsilon_0 + \sqrt{\varepsilon_0}} \right] , \qquad (3.5)$$

$$\Delta E_{\mathbf{k}}^{c} = +e^2 \left[\frac{3}{\pi} \right]^{1/3} \frac{1}{\varepsilon_0} \times \sum_{\mathbf{G},\mathbf{G}'} A_{n\mathbf{k}}^{*}(\mathbf{G}') A_{n\mathbf{k}}(\mathbf{G}) \rho^{1/3}(\mathbf{G}'-\mathbf{G}) - \frac{\mathcal{C}}{2} \left[\frac{\varepsilon_0 - 1}{\varepsilon_0 - \sqrt{\varepsilon_0}} \right] \qquad (3.6)$$

for each band using the electron density and Fourier components of the wave functions generated by the LDA program. This reformulation in terms of $\rho(\mathbf{G})$ allows us to perform more complete calculations than those of Sterne and Inkson,[13,14] who used only the average electron density $\bar{\rho}$. Our approach ensures that proper account is taken of the differing electron densities sampled by the valence- and conduction-band wave functions and so allows us to be more confident in applying these corrections to all the valence bands and a number of the conduction bands. Sterne and Inkson[13] confined their discussion to the highest valence and lowest conduction bands, while Sterne[14] applied the same corrections to all bands. To compute corrections to LDA calculations that go beyond the exchange-only approximation (e.g., including correlation effects) one must simply substitute the correct form for the potential $V_{\text{xc}}^{\text{LDA}}$ in (3.1) and (3.2) and then continue as above. On this basis we have calculated the Sterne-Inkson corrections to both LDA/EX and LDA/CA band structures for a selection of semiconductors and an insulator. Finally, in performing the double summations in (3.5) and (3.6) we terminated each sum at 113 reciprocal-lattice vectors, which is found to be sufficient to give well-converged results.

IV. DISCUSSION OF PRESENT RESULTS

As it has been described in the preceding sections, the Sterne-Inkson model has no remaining adjustable parameters. The quantities a and ε_0 are taken from experiment while $\mathcal{C}$ is estimated in the manner proposed in Sec. II. The values we have used in our calculations are set out in Table I.

The time taken for calculation of the Sterne-Inkson corrections was negligible compared to the time needed for the self-consistent LDA/EX and LDA/CA calculations. The results of our calculations for C, Si, Ge, GaAs, and ZnSe are given in Tables II–VI where they may be compared to those of a number of other workers and to the experimental data. Figure 1 shows the calculated LDA/EX and Sterne-Inkson-corrected band structures for the five materials and clearly reveals the "scissors" nature of the self-energy corrections within the Sterne-Inkson model: the valence bands are hardly altered, while the conduction bands are raised by an almost constant amount regardless of energy or wave vector. This of course reflects the view that the LDA results are likely to be fairly accurate in predicting ground-state properties (i.e., those connected with the valence-band states) and that the error in predicting the conduction bands is largely due to a discontinuity in the exchange-correlation potential at the band gap. It should be stressed that the rigid nature of the corrections is not entirely due to the constant terms in the potentials (i.e., those terms involving $\mathcal{C}$). The contribution from the nonconstant terms is just as large as that from the constant terms and it is the difference between these two contributions that results in the near rigid shift of the conduction bands. In fact the $\mathcal{C}$-dependent terms alone would cause a narrowing of the band gap and it is the nonconstant terms that cause the opening of the gap. It is also interesting to note that the results obtained using the LDA/EX as our starting point and those obtained using the LDA/CA as our starting point are remarkably similar. This is entirely to be expected since the only sense in which the initial LDA calculation should influence the final result is in the closeness of the LDA eigenfunctions to the actual eigenfunctions of the material. Any difference in the LDA eigenvalues is unimportant since the relevant LDA exchange-correlation energy is subtracted from the eigenvalues in (3.1) and (3.2). Both LDA/EX and LDA/CA produce similar eigenfunctions and should, therefore, be expected to yield similar results after correction by the Sterne-Inkson potentials.

Comparing our results with the experimental data we see that good agreement is achieved in diamond, Si, and GaAs whereas in Ge and ZnSe the improvement over the LDA is less conclusive. In a number of ways Si and GaAs are ideal materials for the application of the Sterne-Inkson model. First they have relatively smooth,

TABLE II. LDA and quasiparticle band structures of Si in eV. LDA/EX = LDA with exchange only. LDA/CA = LDA with Ceperley-Alder correlation. n is the band index. Energies have been adjusted to ensure agreement at the top of the valence band.

k	n	LDA/EX	LDA/CA	Present	Hott[a]	HL[b]	ZL[c]	Expt.[a]
Γ	8	3.24	3.27	4.06	3.55	4.08	4.32	4.15
	5–7	2.49	2.54	3.32	3.68	3.35	3.43	3.35
	2–4	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	1	−11.97	−11.93	−11.97	−12.38	−12.04	−12.30	−12.5±0.6
X	7,8	9.99	10.02	10.80	11.67			
	5,6	0.55	0.66	1.39	1.33	1.44	1.47	1.13
	3,4	−2.87	−2.84	−2.87	−2.99	−2.99	−3.02	−2.9
	1,2	−7.80	−7.78	−7.79	−8.15		−8.15	
L	8	7.39	7.57	8.22	8.90			
	6,7	3.26	3.33	4.08	4.38	4.24	4.30	3.91
	5	1.44	1.50	2.27	2.06	2.27	2.36	2.04±0.6
	3,4	−1.21	−1.20	−1.19	−1.15	−1.27	−1.28	−1.2±0.2
	2	−7.02	−6.97	−7.06	−7.39	−7.18	−7.28	−6.8±0.2
	1	−9.62	−9.60	−9.60	−10.04	−9.79	−9.98	−9.3±0.4
E_{gap}	$\Gamma-0.85X$	0.41	0.50	1.25	1.21	1.29	1.32	1.17

[a] Reference 33.
[b] Reference 17.
[c] Reference 36.

shallow, pseudopotentials and so the LDA calculation is likely to be well converged even with a fairly small number of plane waves (i.e., with a low kinetic-energy cutoff). This is important because we rely on the LDA eigenfunctions being close to the actual eigenfunctions of the system, to allow us to perform only one iteration when calculating our corrections. In addition, they have relatively flat extremal bands (as compared to the other materials we have considered) and a relatively constant optical band gap. This means that the highest valence band and lowest conduction band are similar to the pair of flat bands with constant band gap upon which the Sterne-Inkson model is based. In particular, this criterion suggests that, of these two materials, Si appears to be the most suitable, and indeed it is for Si that we find our best results. Whereas the LDA/EX value for the minimum band gap in Si ($\Gamma - 0.8X$) is 0.41 eV, the Sterne-Inkson-corrected figure is 1.25 eV, which is in good agreement with the experimental figure of 1.17 eV. Also the direct band gap at the Γ point shows an improvement from 2.49 to 3.32 eV, which again is very close to the experimental value of 3.35 eV.

In the case of Ge our results show a clear improvement over the LDA but they are not as impressive as in Si or GaAs. For example, the LDA/EX calculation predicts that Ge is a metal with a negative band gap at the Γ point of -0.19 eV while the LDA/CA calculation gives a gap of -0.18 eV. The Sterne-Inkson correction gives us a gap at the Γ point of 0.34 eV which does at least reinstate Ge as a semiconductor, but this is still well below the experimental figure of 0.89 eV. Despite this, the agreement with experiment at other points in the Brillouin zone is reasonably good. The collapse of the lowest LDA conduction band into the valence band at

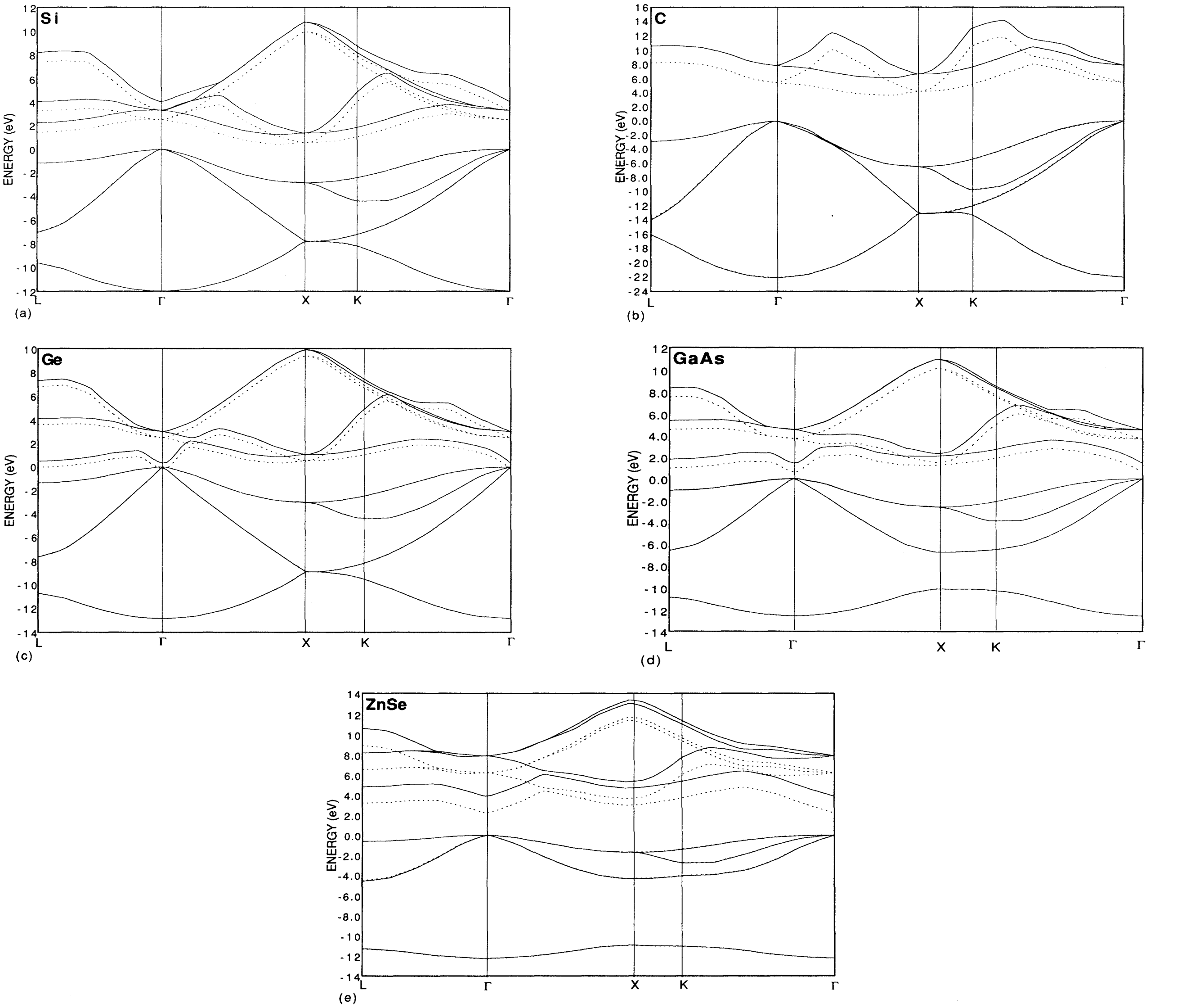

FIG. 1. Pseudopotential quasiparticle band structure (full lines) compared to LDA/EX band structure (dotted lines) for (a) Si, (b) diamond, (c) Ge, (d) GaAs, and (e) ZnSe. Energies in eV refer to the top of the valence band in each case.

TABLE III. LDA and quasiparticle band structures of diamond in eV.

k	n	LDA/EX	Present	Hott[a]	HL[b]	Expt.[a]
Γ	8	13.24	15.65	15.53	14.8	15
	5–7	5.46	7.87	8.84	7.5	7.4
	2–4	0.00	0.00	0.00	0.00	0.00
	1	−22.04	−22.09	−22.77	−23.0	−21
X	5,6	4.19	6.67	7.86		6.0
	3,4	−6.51	−6.52	−6.51		−5
	1,2	−13.10	−13.13	−13.43		−13
L	7	8.61	11.07	11.66		
	5,6	8.24	10.62	11.85		
	3,4	−2.91	−2.88	−2.78		−3
	2	−13.85	−14.00	−14.19	−14.4	−13
	1	−16.08	−16.05	−16.72	−17.3	−16
E_{gap}	$\Gamma-0.7X$	3.76	6.22	7.16	5.6	5.48

[a] Reference 33.
[b] Reference 17.

the Γ point of Ge is well known.[17,33] It may be that this unphysical aspect of the LDA calls into question, at least at the Γ point, the assertion that the LDA wave functions are a sufficiently accurate zeroth-order approximation to the true wave functions. One obvious avenue for further study would be to investigate Sterne-Inkson corrections to calculations carried out beyond the LDA, such as the modified LDA [(M)LDA] of Bylander and Kleinman,[34] in which the collapse may be less severe. Furthermore, our decision to neglect relativistic effects, while probably justified for the other materials considered, is rather more suspect when we are dealing with Ge. Given these difficulties we feel that our results for Ge are quite reasonable and do not cause us to question the validity of the Sterne-Inkson potentials.

In diamond the Sterne-Inkson corrections improve the gap at the Γ point from 5.46 eV in the LDA/EX calculation to 7.87 eV, in fairly good agreement with the experimental figure of 7.4 eV. Similar improvements are obtained across the entire Brillouin zone. Although these results are fairly good, we would like to note in passing that in calculating the basic integrals (2.20) for $\mathcal{C}$ we have used an effective nuclear charge of 3.5, which is probably a quite acceptable figure for most group-IV semiconductors.[29] However, in view of the more compact distribution of valence electrons in diamond it may be reasonable to argue that reduced screening of the nucleus would favor an effective nuclear charge of approximately 4.0 in this case. This would yield a value of $\mathcal{C}=5.1$ eV in diamond, which in turn would lead to corrected results in excellent agreement with experiment. In particular, the gap at the Γ point would become 7.34 eV, while the fundamental indirect gap would be 5.69 eV, as compared with experimental values of 7.4 and 5.48 eV, respectively.

Finally, we note that our results for ZnSe are rather poor, with the band gap overestimated by ~ 1 eV, but this may have less to do with the limitations of the Sterne-Inkson model than with the electronic structure of ZnSe itself. The difficulty here may lie in the fact that Zn has a d band with energy very close to the valence bands of ZnSe. There is, therefore, likely to be significant hybridization of the valence states with these d-band states so that the plane-wave approach used in our LDA program becomes less appropriate. We have treated Zn as a divalent element by assuming the $3d$ electrons to be included in the core and have used the appropriate pseudopotentials.[31] This allows us to take only a 14-Ry cutoff for reasonably converged results but it is not clear if this assumption that the d-band electrons are inert is justified or not.[31] It may also be that our simple method for estimating $\mathcal{C}$, outlined in Sec. II, has broken down in the case of a material whose electronic structure is so far removed from that of diamond.

TABLE IV. LDA and quasiparticle band structures of Ge in eV.

k	n	LDA/EX	LDA/CA	Present	Hott[a]	HL[b]	Expt.[b]
Γ	6–8	2.49	2.54	3.03	3.60	3.04	3.01
	5	−0.19	−0.18	0.34	0.06	0.71	0.89
	2–4	0.00	0.00	0.00	0.00	0.00	0.00
	1	−12.8	−12.80	−12.82	−13.16	−12.86	−12.6
X	7,8	9.40	9.43	9.94	10.96		
	5,6	0.52	0.64	1.07	1.31	1.23	1.3±0.2
	3,4	−3.03	−3.00	−3.03	−3.26	−3.22	−3.15±0.2
	1,2	−8.91	−8.90	−8.91	−9.31	−9.13	−9.3±0.2
L	8	6.80	7.00	7.35	8.30	7.61	7.8±0.6
	6,7	3.61	3.69	4.14	4.73	4.33	4.3±0.2
	5	−0.03	0.04	0.51	0.59	0.75	0.744
	3,4	−1.37	−1.36	−1.37	−1.36	−1.43	−1.4±0.3
	2	−7.61	−7.57	−7.64	−8.06	−7.82	−7.7±0.2
	1	−10.72	−10.71	−10.71	−11.12	−10.89	−10.6±0.5
E_{gap}	$\Gamma-L$	−0.03	0.04	0.51	0.59	0.75	0.744

[a] Reference 33.
[b] Reference 17.

TABLE V. LDA and quasiparticle band structures of GaAs in eV.

k	n	LDA/EX	LDA/CA	Present	Hott[a]	WGL[b]	ZL[c]	Expt.[b]
Γ	6–8	3.70	3.76	4.52	4.72	4.55		4.716
	5	0.61	0.65	1.43	0.93	1.42	1.22	1.522
	2–4	0.00	0.00	0.00	0.00	0.00		0.00
	1	−12.59	−12.56	−12.59	−12.94	−13.06		−13.1
X	7,8	10.14	10.18	10.96	11.79	11.06		
	6	1.50	1.61	2.32	2.24	2.26		2.58
	5	1.26	1.41	2.10	1.99	1.98		2.08
	3,4	−2.62	−2.589	−2.63	−2.89	−2.82		−2.80
	2	−6.76	−6.72	−6.78	−7.64	−7.12		−6.70
	1	−10.15	−10.149	−10.13	−10.28	−10.33		−10.75
L	8	7.52	7.718	8.35	8.95			
	6,7	4.53	4.62	5.35	5.63	5.40		
	5	0.97	1.048	1.78	1.40	1.72		1.85
	3,4	−1.10	−1.09	−1.11	−1.13	−1.21		−1.30
	2	−6.60	−6.54	−6.63	−7.41	−6.87		−6.70
	1	−10.91	−10.90	−10.89	−11.14	−11.29		−11.24
E_{gap}	Γ−Γ	0.61	0.65	1.43	0.93	1.42	1.22	1.522

[a] Reference 33.
[b] Reference 35.
[c] Reference 36.

V. COMPARISON WITH PREVIOUS WORK

One of the most successful applications of the self-energy concept to the problem of band-structure calculation is the following method due to Hybertsen and Louie.[17] The static dielectric matrix $\varepsilon_{\mathbf{GG}'}(\mathbf{q},\omega=0)$ is dependent only on ground-state properties of the system and so can be accurately calculated within the density-functional theory. The resulting matrix is then extended to the finite frequency case by means of a generalized-plasmon-pole model (GPP) in which the dynamic structure of the dielectric matrix is modeled by a pair of simple poles for each element of the matrix. The precise nature of these poles is then fixed by requiring that the dielectric matrix satisfies the Kramer-Krönig relation

$$\mathrm{Re}\,\varepsilon_{\mathbf{GG}'}(\mathbf{q},\omega=0)=\delta_{\mathbf{GG}'}+\frac{2}{\pi}P\int_0^{\infty}d\omega\frac{1}{\omega}\mathrm{Im}\,\varepsilon^{-1}_{\mathbf{GG}'}(\mathbf{q},\omega) \tag{5.1}$$

and the generalized f-sum rule

$$\int_0^{\infty}d\omega\,\omega\,\mathrm{Im}\,\varepsilon^{-1}_{\mathbf{GG}'}(\mathbf{q},\omega)=-\frac{\pi}{2}\omega_p^2\frac{(\mathbf{q}+\mathbf{G})\cdot(\mathbf{q}+\mathbf{G}')}{|\mathbf{q}+\mathbf{G}|^2}\frac{\rho(\mathbf{G}-\mathbf{G}')}{\rho(\mathbf{0})}\ . \tag{5.2}$$

Energy-dependent expressions for the screened exchange and Coulomb hole contributions to the self-energy are then obtained within the GW approximation and the eigensolutions of the system are evaluated, using LDA eigenfunctions as a starting point. Note that this involves the numerical evaluation of the frequency integration from (1.1), a step that is performed analytically within the Sterne-Inkson model. This is part of the reason for the relative speed of the calculations that we have made. The results generated by Hybertsen and Louie using the GPP model for C, Si, Ge, and LiCl match the experimental results very closely. In particular, we note that the figures quoted for Ge and diamond are much better than our own, although in the case of Si there is quite close agree-

TABLE VI. LDA and quasiparticle band structures of ZnSe in eV.

k	n	LDA/EX	LDA/CA	Present	Expt.[a]
Γ	6–8	6.20	6.30	7.77	7.33
	5	2.21	2.33	3.77	2.82[b]
	2–4	0.00	0.00	0.00	0.00
	1	−12.27	−12.26	−12.26	−12.25
X	8	11.69	11.79	13.27	
	7	11.40	11.51	12.93	
	6	3.66	3.79	5.22	5.17
	5	2.99	3.19	4.59	4.54
	3,4	−1.69	−1.66	−1.71	−1.96
	2	−4.33	−4.27	−4.37	−4.96
	1	−10.79	−10.99	−10.95	−10.72
L	8	8.88	9.07	10.47	
	6,7	6.51	6.64	8.05	7.72
	5	3.19	3.31	4.70	3.96
	3,4	−0.62	−0.61	−0.62	−0.76
	2	−4.54	−4.47	−4.63	−5.08
	1	−11.35	−11.35	−11.32	−11.08
E_{gap}	Γ−Γ	2.21	2.33	3.77	2.82[a]

[a] Reference 40.
[b] Reference 30.

ment. Additionally there is good agreement between our figures for GaAs and those produced by Wang, Gu, and Li,[35] who have performed calculations using the GPP model for both GaAs and GaP. Recently Zhu and Louie[36] have obtained good results using the GPP approach but starting with a model static dielectric matrix. Use of a model in evaluating the static matrix simplifies the most time consuming step of their calculation, but their results for Si and GaAs are not as close to experiment as ours. The ability of any simple GPP model to accurately represent the dynamic effects in the dielectric matrix has recently been questioned,[18,19] but nevertheless the excellent results obtained by these workers strongly suggest that a complete self-energy calculation of some sort is indeed the correct approach to the solution of the band-structure problem.

An alternative to the GPP technique is the dielectric band-structure (DBS) approach developed by Baldereschi and Tosatti.[37] In the context of *GW* calculations this method has been used by von der Linden and Horsch[38] and by Hott.[33] In essence the crucial step is the diagonalization of the dielectric matrix, yielding a set of eigenvectors and eigenvalues. There are an infinite number of eigenvalues for each point in the Brillouin zone, forming an infinite set of dielectric bands lying in the range (0,1). Inversion of the dielectric matrix is simply achieved by inverting the eigenvalues and the energy dependence of the screening is then introduced by means of a plasmon-pole function for each eigenvalue. As before, the parameters for the pole structure are found through the f-sum rule, but there are fewer parameters required than in the GPP model in which every matrix element was parametrized. Certainly the analytic structure achieved in this way is different from that of the GPP method but it is not clear which may be considered to be closest to the actual structure. In computing the self-energy within this model a sum over the dielectric bands must be performed instead of the sum over reciprocal-lattice vectors involved in the GPP method. The sum over dielectric bands is expected to converge more rapidly[38] and this is another advantage of the DBS technique. However, the quasiparticle energies obtained by Hott using this method are not as impressive as those of Hybertsen and Louie. Indeed, the results of our own much simpler calculations match those of Hott fairly closely for Si while they are markedly closer to the experimental data for GaAs, Ge, and diamond. The root of the problem may lie in the partition of information between the eigenvectors and eigenvalues in the dielectric band-structure formalism. In the GPP model it is clear that every element of the dielectric matrix satisfies the f-sum rule, yet in the DBS model it is only the eigenvalues which satisfy it. Although the eigenvalues contain much of the information about the dielectric matrix, they do not completely describe it and so merely considering the pole structure of the eigenvalues does not guarantee that the pole structure of the full matrix will be reproduced. The GPP model evidently produces better results but the drawback is the need to calculate a large number of parameters compared to the DBS method. Additionally, the use of empirical pseudopotentials in Hott's method is not entirely satisfactory as it does not allow truly *ab initio* self-energy corrections to be evaluated.

Recent calculations have been made by Bechstedt *et al.*[39] using a simple static model for the dielectric function and introducing dynamic screening and local-field effects through two parameters. Their results are comparable with ours for Si, GaAs, and ZnSe. However, although their scheme vastly reduces the computer time required to calculate the self-energy, their LDA calculations are based upon empirically obtained local pseudopotentials and so their work does not have the same firm basis as our own.

Finally, we must mention the work of Hanke and Sham.[15] The model that they have proposed is of a very similar nature to the earlier work of Sterne and Inkson, in that it is based upon a pair of tight-biding bands and leads to a pair of local potentials dependent upon $\rho^{1/3}(\mathbf{r})$. In this model the screened interaction is represented by a very simple plasmon-pole-type expression. Performing the frequency integration in the finite temperature form they partition the self-energy into three contributions: a bare exchange term, an antibonding correlation term, and a bonding correlation term. Local expressions for the valence- and conduction-band self-energies are then found through a number of approximations and their matrix elements are evaluated using wave functions obtained from a LDA calculation. Full quasiparticle band structures were not presented, but their matrix elements varied significantly from those which Hybertson and Louis give.[17] Nevertheless, the value of Δ, the discontinuity in the DFT exchange-correlation potential (also known as the gap correction), is accurately reproduced by their model when compared to first-principles calculations by Godby, Schlüter, and Sham[9] for both diamond and Si. However, the quantity Δ on its own is of little practical use since it does not represent the correction to be applied to a LDA calculation but rather to a "true" DFT (Ref. 9) calculation, which was not attempted within this model.

VI. SUMMARY

In this paper we have reviewed the tight-binding model proposed by Sterne and Inkson[13,14] for the evaluation of the self-energy operator and have presented the results of calculations based on this model for a range of materials from the narrow-gap semiconductor Ge to the insulator diamond. We have found that the results from this simple scheme for diamond, Si, and GaAs are particularly impressive, while those for Ge and ZnSe have been less so. We believe that we have shown this model to be useful in providing a simple method for calculating many-body effects in semiconductors and insulators whose extremal bands are relatively flat and which exhibit a fairly constant optical band gap. At its best, the Sterne-Inkson model provides results that are at least as good as those of any other more detailed calculation, but at a considerably lower computational cost. Having shown that the present scheme gives the correct bulk limits, we will expect it to be very valuable in large-scale applications to situations where a real-space self-energy description would be beneficial (e.g., low-dimensional systems). Work on such applications will be presented in a future publication.

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