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Elimination of unoccupied state summations in *ab initio* self-energy calculations for large supercells

Lucia Reining
Laboratoire des Solides Irradiés, URA 1380 CNRS - CEA/DTA/DECM Ecole Polytechnique, F-91128 Palaiseau, France

Giovanni Onida
Laboratoire des Solides Irradiés, URA 1380 CNRS - CEA/DTA/DECM Ecole Polytechnique, F-91128 Palaiseau, France and Istituto Nazionale per la Fisica della Materia, Dipartimento di Fisica dell'Università di Roma Tor Vergata, Via della Ricerca Scientifica, I–00173 Roma, Italy

R.W. Godby
Department of Physics, University of York, York YO1 5DD, United Kingdom

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We present a new method for the computation of self-energy corrections in large supercells. It eliminates the explicit summation over unoccupied states, and uses an iterative scheme based on an expansion of the Green's function around a set of reference energies. This improves the scaling of the computational time from the fourth to the third power of the number of atoms for both the inverse dielectric matrix and the self-energy, yielding improved efficiency for 8 or more silicon atoms per unit cell.

The quasiparticle (QP) band structure of a system of interacting electrons (the single-particle-like approximate eigenstates which describe the addition of an electron or a hole) is obtained from solutions of a Schrödinger equation in which exchange and correlation is described by the electron self-energy Σ. *Ab initio* calculations of QP energies for real solids have been performed since the 1980s [e.g. [1–3]], generally using two approximations: (i) the self-energy is evaluated within Hedin's GW approximation [4], where it is described as the convolution of the one-particle Green's function G and the screened Coulomb interaction W, both of which are obtained from an initial density-functional-theory (DFT) calculation using the local-density approximation (LDA); and (ii) the QP energies are evaluated in first-order perturbation theory, starting from the DFT-LDA eigenvalues and eigenstates. Band structures in excellent agreement with experiments have been obtained in this way for many systems, but the applications are at present restricted to relatively small basis sets and unit cells: calculating the inverse dielectric matrix and the QP energies is computationally demanding, and scales essentially as N_{at}^4, the fourth power of the number of atoms in a supercell. The potential applications of *ab initio* electronic-structure calculations are therefore restricted in comparison with ground-state calculations.

A recent real-space-imaginary-time approach [5] scales as N_{at}^2 for the construction of the Green's function and as N_{at} for the formation of the dielectric matrix and self-energy. However, the method is designed for calculations that require the whole self-energy $\Sigma(\mathbf{r}, \mathbf{r}', \omega)$ for all $\mathbf{r}$ and $\mathbf{r}'$, and, for feasible system sizes, is less efficient if only

a few matrix elements of Σ are required. A mixed-space approach [6] for the dielectric matrix scales as N_{at}^3, but does not address the construction of the self-energy. In this paper we describe a new approach that yields efficient calculation of QP energies for supercells of the order of 10-100 atoms.

In the past, considerable progress has been made in the calculation of the single-particle time-ordered response function χ_0,

$$\chi^0{}_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) = \frac{2}{\Omega}\sum_{nn'\mathbf{k}}(f_{n\mathbf{k}'} - f_{n'\mathbf{k}})\frac{\langle n\mathbf{k}'|e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|n'\mathbf{k}\rangle\langle n'\mathbf{k}|e^{i(\mathbf{q}+\mathbf{G}')\cdot\mathbf{r}'}|n\mathbf{k}'\rangle}{(E_{n\mathbf{k}'} - E_{n'\mathbf{k}} + \omega + i\eta\cdot sgn\,(E_{n'\mathbf{k}} - E_{n\mathbf{k}'}))} \tag{1}$$

where $\mathbf{k}' = \mathbf{k} - \mathbf{q}$, n and n' run over the bands, the $f_{n'\mathbf{k}}$ are occupation numbers, $|n\mathbf{k}'\rangle$ are the one-electron eigenfunctions calculated, for instance, using the local-density approximation, and Ω is the volume of the unit cell. Based on the perturbation summation approach of Dalgarno and Lewis [7], Baroni and co-workers [8,9] have designed a Green's-function approach which avoids the explicit summation over unoccupied states in (1) for the case of static response; their method has recently been generalized to the dynamical χ_0 [10]. It is hence a natural idea to extend those advantages to self-energy calculations, in which χ_0 is the main ingredient for the determination of the inverse dielectric matrix $\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$, and a second sum over empty states, arising from the Green's function G, appears in the expression for the matrix elements of Σ. At first sight the matrix elements of Σ are formally similar to χ_0, especially in a plasmon-pole approximation such as that of Ref. [11]: essentially, (1) has to be modified by some $(\mathbf{G},\mathbf{G}')$-dependent prefactors, and ω substituted by the plasmon-pole parameters $\tilde{\omega}_{\mathbf{G}\mathbf{G}'}$ (see later). However, two main obstacles hinder the extension of the approach to self-energy calculations. First, when all matrix elements $(\mathbf{G},\mathbf{G}')$ of χ_0 are needed, as is the case in QP calculations, the straightforward application of the method proposed in Ref. [10] to χ_0 still yields an N_{at}^4 scaling: this is because the method requires a matrix inversion, which scales as N_{at}^3, for each of the N_v energy denominators appearing in (1), where N_v, the number of valence states, is obviously proportional to N_{at}. In the case of $\langle\Sigma\rangle$ the situation is even worse, since the number of different energy denominators is proportional to N_v times the number of different plasmon pole frequencies $\tilde{\omega}_{\mathbf{G}\mathbf{G}'}$, one for each (G,G') pair. The scaling would be in this case N_{at}^6!

Here we propose an extension of the Green's-function technique to the calculation of self-energy corrections which maintains its advantages, and moreover has the improved scaling of N_{at}^3 (ignoring log N_{at} contributions) for both $\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$ and $\langle\Sigma\rangle$, together with a favourable prefactor. Our approach is based on Taylor expansions of the Green's functions, which are shown to converge rapidly, keeping the same numerical stability and controllability as the commonly used empty-states summation method. We illustrate the performance of our method for the example of successively large supercells of bulk sili-

con, showing that quasiparticle calculations in the framework of the standard GW approach [2–4,11] for systems such as point defects or amorphous silicon are made feasible.

We start from the Green's-function idea of Ref. [8,10] for the calculation of χ_0 in (1), where the solution of the linear system

$$(-H + E_{v\mathbf{k}'} \pm \omega + i\eta)\,|\Psi^{\pm}_{v,\mathbf{k}',\mathbf{q},\mathbf{G}',\omega}\rangle = e^{i(\mathbf{q}+\mathbf{G}')\cdot\mathbf{r}}|v\mathbf{k}'\rangle \tag{2}$$

for the "polarization state" $|\Psi^{\pm}_{v,\mathbf{k}',\mathbf{q},\mathbf{G}',\omega}\rangle$ allows to rewrite χ_0 as

$$\chi^0_{\mathbf{G}\,\mathbf{G}'}(\mathbf{q},\omega) = \frac{2}{\Omega}\sum_{\mathbf{k}\,v}\langle v,\mathbf{k}'|e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}(|\Psi^+\rangle + |\Psi^-\rangle) \tag{3}$$

As above, $|v\mathbf{k}\rangle$ is the LDA Bloch function $e^{i\mathbf{k}\cdot\mathbf{r}}u_{v,\mathbf{k}}(\mathbf{r})$, $\mathbf{k}' = \mathbf{k} - \mathbf{q}$, and H is the LDA Hamiltonian.

When ω tends to zero, $(-H+E_{v,\mathbf{k}}\pm\omega+i\eta)^{-1}$ diverges, as do $|\Psi^+\rangle$ and $|\Psi^-\rangle$. However, the sum (3) remains finite, since $\langle\Psi^-_{v',\mathbf{k},-\mathbf{q},-\mathbf{G}',\omega}|v\mathbf{k}'\rangle = -\langle v'\mathbf{k}|\Psi^+_{v,\mathbf{k}',\mathbf{q},\mathbf{G}',\omega}\rangle$. For numerical stability, it is then better to project out the valence states from H since the beginning, in a way similar to that of ref. [8]: we change the operator H appearing on the left side of Eq. (2) into $\tilde{H} = HP$ where $P = 1 - \sum_v |v\rangle\langle v|$, and we modify the right–hand side of Eq. (3) inserting the projector P to the left of both Ψ^+ and Ψ^-.

We write (2) in reciprocal space as

$$\sum_{\mathbf{G}''}\left(-\tilde{H}_{\mathbf{k}+\mathbf{G},\mathbf{k}+\mathbf{G}''} + (E_{v,\mathbf{k}'} \pm \omega + i\eta)\delta_{\mathbf{G},\mathbf{G}''}\right) f^{\pm}_{\mathbf{G}''}(v,\mathbf{k}',\mathbf{q},\mathbf{G}',\omega) = u_{\mathbf{G}-\mathbf{G}'}(v,\mathbf{k}') \tag{2b}$$

where $f^{\pm}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\Psi^{\pm}_{v,\mathbf{k}',\mathbf{q},\mathbf{G}',\omega}(\mathbf{r})$ is a periodic function in $\mathbf{r}$. An LU decomposition (or inversion) of $(-\tilde{H} + E_v \pm \omega + i\eta)$ scales as N^3 with the number of plane waves, N, for every valence energy E_v, yielding the N^4_{at} scaling of the "naïve" implementation. Then, the solution for each right-hand side requires N^2 operations for every G' and every $u_{v,\mathbf{k}'}$ (or $N^2 logN$ operations for every $u_{v,\mathbf{k}'}$ and the whole set of G', when fast Fourier transforms (FFTs) are used).

Equation (3) becomes

$$\chi^0_{\mathbf{G}\,\mathbf{G}'}(\mathbf{q},\omega) = \frac{2}{\Omega}\sum_{v\mathbf{k}'}\int d\mathbf{r}\;\; u^*_{v,\mathbf{k}'}(\mathbf{r})e^{-i\mathbf{G}\cdot\mathbf{r}}(f^+_{\mathbf{r}}(v,\mathbf{k}',\mathbf{q},\mathbf{G}',\omega) + f^-_{\mathbf{r}}(v,\mathbf{k}',\mathbf{q},\mathbf{G}',\omega)), \tag{3b}$$

which is again computed efficiently using FFTs. Before coming to the possible improvements in the calculation of χ_0, it is useful to look directly at the self-energy matrix elements. The main numerical effort lies in the evaluation of the correlation contribution, which is

$$\begin{aligned}\langle n\mathbf{k}|\Sigma_c(\omega)|n\mathbf{k}\rangle = &\frac{2\pi}{N\Omega}\sum_{c'\mathbf{k}'}\sum_{\mathbf{G}\mathbf{G}'}\frac{\Omega^2_{\mathbf{G}\mathbf{G}'}}{|\mathbf{q}+\mathbf{G}||\mathbf{q}+\mathbf{G}'|}\frac{\langle n\mathbf{k}|e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|c'\mathbf{k}'\rangle\langle c'\mathbf{k}'|e^{i(\mathbf{q}+\mathbf{G}')\cdot\mathbf{r}'}|n\mathbf{k}\rangle}{\tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})\,(\omega - \tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) - E_{c'\mathbf{k}'})} \\ &+ \frac{2\pi}{N\Omega}\sum_{v'\mathbf{k}'}\sum_{\mathbf{G}\mathbf{G}'}\frac{\Omega^2_{\mathbf{G}\mathbf{G}'}}{|\mathbf{q}+\mathbf{G}||\mathbf{q}+\mathbf{G}'|}\frac{\langle n\mathbf{k}|e^{-i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|v'\mathbf{k}'\rangle\langle v'\mathbf{k}'|e^{i(\mathbf{q}+\mathbf{G}')\cdot\mathbf{r}'}|n\mathbf{k}\rangle}{\tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})\,(\omega + \tilde{\omega}_{\mathbf{G}\mathbf{G}'}(\mathbf{q}) - E_{v'\mathbf{k}'})}\end{aligned} \tag{4}$$

where $\mathbf{k}' = \mathbf{k} - \mathbf{q}$, $\Omega_{\mathbf{GG}'}$ and $\tilde{\omega}_{\mathbf{GG}'}$ are the plasmon-pole parameters determined by the energy dependence of $\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$, and c' (v') denote sums over unoccupied (occupied) states. Because of the sum over unoccupied states, the first of the two terms is the computationally demanding one. Contrarily to eq.(1), here there is a different energy denominator for each plasmon–pole frequency, $\tilde{\omega}_{\mathbf{GG}'}$. As pointed out above, performing a new LU decomposition (or inversion) for each individual (G,G') pair would lead to an N_{at}^6 scaling, making the approach disadvantageous even with respect to the traditional method. However,it is known that $\Sigma(\omega)$ is a smooth function of ω, which implies that it might also be a smooth function of $\omega - \tilde{\omega}_{\mathbf{GG}'}$. We observe that many of the N^2 different $\tilde{\omega}_{\mathbf{GG}'}$ have similar values, and that ω is typically taken at the DFT eigenvalue of state $|nk\rangle$; it is therefore possible to evaluate the contributions from different $\tilde{\omega}_{\mathbf{GG}'}$ by means of a Taylor expansion of $(\omega - \tilde{\omega}_{\mathbf{GG}'} - \tilde{H})^{-1}$ around $\omega - \tilde{\omega}_{\mathbf{GG}'} = E_{n,0} - \tilde{\omega}_0$, for one or more expansion points $E_{n,0}$ and $\tilde{\omega}_0$ in the range of interest. Since the width of the energy interval into which the E_n of interest and the plasmon pole parameters $\tilde{\omega}_{\mathbf{GG}'}$ are scattered does not grow with the system size, the number of expansion points needed – and hence the number of matrix inversions – no longer depends on N_{at}.

Expression (4) also contains possibly divergent contributions, which could hinder the application of the Green's-function approach to the first term: when $\mathrm{E}_{c'\mathbf{k}'}$ is an unoccupied state, divergences arise for $\omega - E_{c'\mathbf{k}'} = \tilde{\omega}$, hence when ω is at an energy at least $\tilde{\omega}_{\mathbf{GG}'}$ *above* the lowest conduction state. In order to avoid such divergences, we divide the unoccupied states into two groups: the 'low–lying' states with energies from the Fermi energy to somewhat beyond the highest quasiparticle energy of interest, and the states with higher energies. Then we apply the Green's-function trick to the latter states only, now including the low–lying states in the projector P, making the solution well defined for all the energies in the range of interest.

The Taylor coefficients, i.e. the energy derivatives of $\tilde{G}(\tilde{\omega}) = (-HP + E_{0,n} - \tilde{\omega})^{-1}$, are essentially powers of $\tilde{G}(\tilde{\omega}_0)$. Then, their computation only requires as many matrix multiplications as the order of the expansion (typically 1 or 2). The contributions of the different orders can be evaluated separately, in a CPU time proportional to N_{at}^3 [12]. The derivative $\langle \partial\Sigma/\partial\omega \rangle$, used in calculating $\langle n|\Sigma(\omega)|n\rangle$ as $\langle n|\Sigma(E_n^{DFT})|n\rangle + \langle \partial\Sigma/\partial\omega\rangle \cdot (\omega - E_n^{DFT})$ (see Ref. [11]), is also determined by the second power of $\tilde{G}$, and hence does not require any further effort. The only term whose evaluation is in principle still proportional to N_{at}^4 is the summation over the occupied and lowest unoccupied states, which is performed explicitly. However, the actual number of operations involved is negligible, since the number of these low–lying states is small.

The expansion approach can be used in the same way to improve the calculation of $\chi_0(\omega)$. Here there are in

principle as many different energies in the denominator as valence states. Using the expansion technique, one only has to compute $(-\hat{H} + E_{v0} + \omega)^{-i}$ for a number of expansion points E_{v0} which is proportional to the width of the valence band (independent of system size). In the case of χ_0 for silicon, inclusion of orders $(i-1)$ from 0 to 3 is sufficient to achieve an accuracy of about 50 meV in $\langle\Sigma\rangle$, using 3 expansion points.

To demonstrate that the method is well suited to *ab initio GW* calculations for large unit cells with many electrons, we have computed the *GW*-corrected electronic structure for different supercells of bulk silicon, using the Γ point only. In Table I, we illustrate for the 2-atom cell the good convergence of single elements of ϵ^{-1} with the order of the Taylor expansion. "Exact" results are obtained by using the traditional method, with 181 plane waves (which corresponds to the 12.5 Ry energy cutoff used in the DFT calculation) and the whole 181 states. Table II shows the results for the matrix elements of Σ as a function of the order of its Taylor expansions (using a 3rd order expansion for ϵ^{-1} throughout). We compare with the exact results and with the approximate results which are obtained with the traditional approach, using 169 plane waves and 112 states. The 'traditional' results have an accuracy of 50 meV, and, with our method, inclusion of orders 0, 1 and 2 are seen to be sufficient to achieve the same accuracy.

The computational time as a function of the supercell size is illustrated in Fig. 1. To allow a fair comparison, both calculations have been performed with the parameters leading to an accuracy of about 50 meV. The two approaches are already equivalent for an 8-atom silicon supercell. With 54 atoms the new method gains a factor of five in computing $\langle\Sigma\rangle$; here the CPU time required to compute the dielectric function, plus Σ and its energy derivative for all 66 states lying within 0.1 Hartrees of the Fermi energy is 42 hours on a Cray C98 computer, 22 hours of which is for χ_0. This means that quasiparticle calculations in the framework of the standard *GW* approximation for systems such as point defects or amorphous silicon are feasible with a reasonable computational effort. We have already successfully applied the present approach to the calculation of χ_0 and $\langle\Sigma\rangle$ for sodium clusters in a large supercell [13].

A possible improvement, which will reduce the computational effort further, is to exploit the fact that in our scheme, by analogy with what is pointed out in Ref. [5] and [6], we compute quantities which are short-ranged in $(\mathbf{r} - \mathbf{r}')$. Introducing a real-space cutoff in $(-HP + \omega - \tilde{\omega})^{-1}$ will reduce the computational expense significantly (at present, without the cutoff, FFTs account for more than half of the total CPU time.)

In summary, we have introduced a scheme which extends towards larger sizes and complexity the set of physical systems for which self-energy-corrected electronic structure can be computed, within Hedin's *GW* scheme and the plasmon-pole approximation. By avoiding the need for an explicit summation over conduction states,

and introducing an iterative scheme to describe the energy dependence of the Green's function by expanding around a few reference energies, the method reduces the scaling of the computational time from N_{at}^4 to N_{at}^3. Systems with a number of atoms N_{at} of the order of 50, which would require a prohibitive computational effort within traditional GW schemes, thereby become accessible. The present method appears to be a promising tool for the study of complex structures such as clusters, reconstructed surfaces, and point defects in semiconductors, since they often fall within this class of systems.

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[1] G. Strinati, H. J. Mattausch, and W. Hanke, Phys Rev. B **25**, 2867 (1982).
[2] M.S. Hybertsen and S.G. Louie, Phys. Rev. Lett. **55**, 1418 (1985), Phys. Rev. **B 34**, 5390 (1986).
[3] R.W. Godby, M. Schlüter, and L.J. Sham, Phys. Rev. Lett. **56**, 2415 (1986); Phys Rev. B **37**, 10159 (1988).
[4] L. Hedin, Phys. Rev. **139**, 796 (1965).
[5] H.N. Rojas, R.W. Godby, and R.J. Needs, Phys. Rev. Lett. **74** , 1827 (1995).
[6] X. Blase, A. Rubio, S.G. Louie, and M. Cohen, Phys. Rev. B. **52**, R2225, (1995).
[7] A. Dalgarno and J.T. Lewis, Proc. R. Soc. London **A 233**, 70 (1955).
[8] S. Baroni and A. Quattropani, Il Nuovo Cimento **5D**, 89 (1985).
[9] S. Baroni, P. Giannozzi, and A. Testa, Phys. Rev. Lett. **58**, 1861 (1987).
[10] A.A. Quong and A.G. Eguiluz, Phys. Rev. Lett. **70**, 3955 (1993).
[11] R.W. Godby and R.J. Needs, Phys. Rev. Lett. **62**, 1169 (1989).
[12] Matrix multiplications are performed using the Strassen algorithm, which scales as $N^{2.8}$ rather than N^3.
[13] G. Onida, L. Reining, R.W. Godby, R. Del Sole, and W. Andreoni, Phys. Rev. Lett. **75**, 818 (1995).

TABLE I. Typical convergence of $(\mathbf{G}, \mathbf{G}')$ elements of ϵ^{-1} with the order of the Taylor expansion (see text).

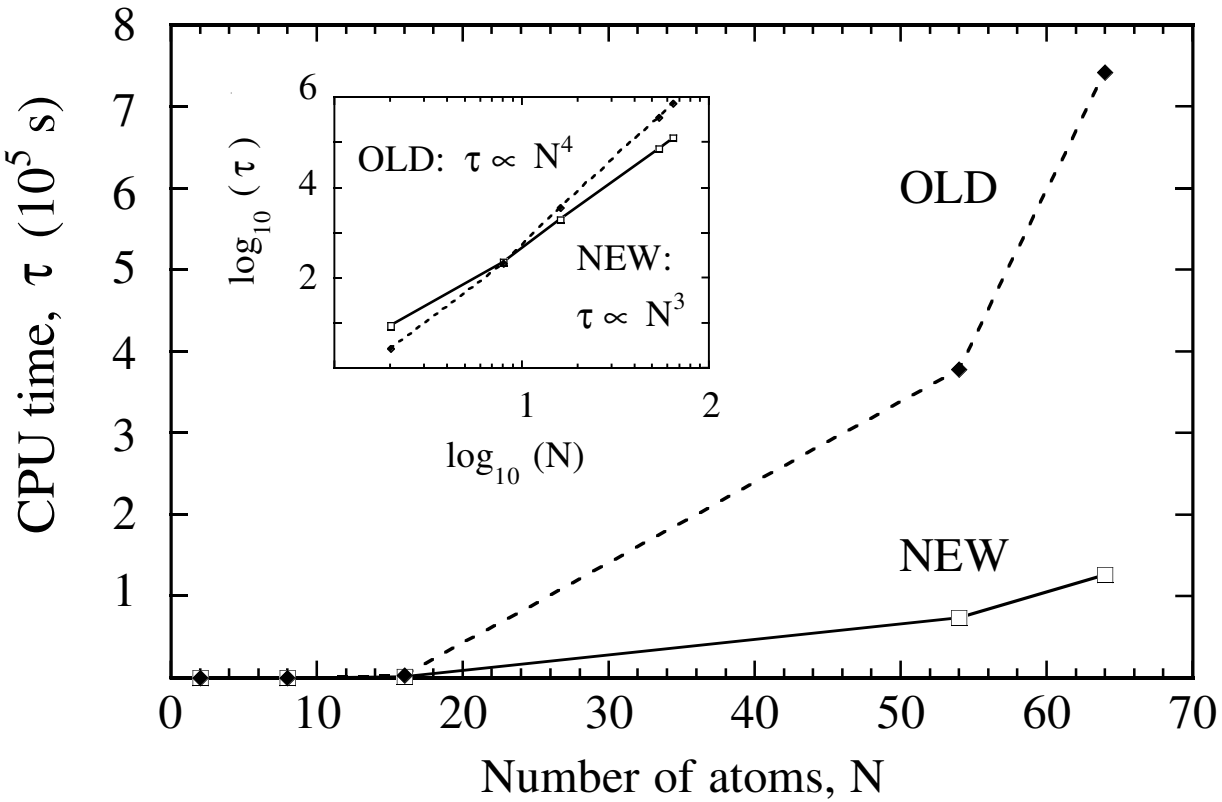
G	**G'**	order 0	1	2	3	4	5	6	7	exact
(000)	(000)	0.0347	0.0121	0.0082	0.0069	0.0064	0.0061	0.0060	0.0060	0.0059
$(\bar{1}1\bar{1})$	$(\bar{1}1\bar{1})$	0.6373	0.6197	0.6138	0.6121	0.6114	0.6112	0.6111	0.6110	0.6110
$(00\bar{2})$	$(00\bar{2})$	0.6336	0.5998	0.5879	0.5833	0.5812	0.5802	0.5797	0.5794	0.5792
(111)	$(00\bar{2})$	-0.0215[a]	-0.0231[a]	-0.0240[a]	-0.0244[a]	-0.0246[a]	-0.0247[a]	-0.0247[a]	-0.0248[a]	-0.0248[a]
$(3\bar{1}1)$	$(\bar{3}1\bar{1})$	0.0131[b]	0.0167[b]	0.0183[b]	0.0190[b]	0.0193[b]	0.0195[b]	0.0195[b]	0.0196[b]	0.0196[b]

[a] times $1 - i$
[b] times i

TABLE II. Quasiparticle corrections to the LDA eigenvalues for bulk silicon, calculated with the present method for different orders of the Taylor expansion for Σ (columns 1, 2 and 3), and with the traditional method summing over *all* the conduction states (for the chosen plane-wave basis set) (column 4), and summing over about 2/3 of the conduction states (column 5). Values in eV.

	1^{st} ord.	2^{nd} ord.	3^{rd} ord.	"Exact"	Trad.
Γ'_{25v}	0.080	0.030	0.020	-0.013	0.035
Γ_{15c}	0.576	0.515	0.498	0.485	0.530
Γ'_{2c}	0.692	0.605	0.575	0.553	0.582

FIG. 1. CPU time required for the calculation of the *GW* corrections to the LDA electronic structure, as a function of the number of atoms in the supercell. Filled diamonds are for the traditional method, hollow squares for the present scheme. In the inset, a log-log plot of the same variables shows the cross-over at the 8 atom supercell.


CPU time, τ (10^5 s)
Number of atoms, N
OLD
NEW
OLD: τ ∝ N^4
NEW: τ ∝ N^3
log10 (τ)
log10 (N)