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Calculation of extended electronic states in simple liquids and plasmas

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The calculation of some electronic processes, such as bound-free transitions in plasmas, require a description of the free-electron wave function that is consistent with that of the bound state. Because the plasma is a disordered media, such a description is difficult. In this paper, we first propose that the one-electron expectation values $\langle \psi_E|A|\psi_E\rangle$ can be considered as self-averaging quantities when $|\psi_E\rangle$ is delocalized. Using this, we give a description of the eigenstate that is consistent with the disorder, and that permits us to calculate $\langle \psi_E|A|\psi_E\rangle$ in the thermodynamic limit. Finally, we test the method by calculating an electron-ion correlation function in liquid sodium. [S1063-651X(96)03608-2]

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I. INTRODUCTION

An electronic property can be computed as the expectation value of a relevant operator [i.e., $\mathrm{Tr}(\rho A)$]. Over the past 30 years, powerful operatorial methods have been developed to calculated these expectation values independently from the eigenstates [1,2]. These methods, however, are not convenient to calculate the detailed absorption spectrum that is useful in opacity calculations [3]. For this problem, a better accuracy is obtained by expanding the relevant operator in terms of the electron wave functions. The averaged bound-free transition elements, for example, are calculated using the wave functions of the bound and of the free states. However, the free-electron wave function is usually obtained from a spherically averaged potential [4–6], and this is not satisfying when the system is disordered and when the density is large. Hence a better method to calculate such quantities would be useful, and this is the motivation of the present work.

Considering a delocalized eigenstate of energy E (in place of a free state, which would be relevant to a spherical potential), we examine the quantity $\langle \psi_E|A|\psi_E\rangle$, where A is an operator. For example, within the electric dipolar approximation, the averaged transition matrix element from the bound orbital $|\varphi\rangle$ to a state at energy E is proportional to

$$\sum_{|\psi_E\rangle} \langle \psi_E|A|\psi_E\rangle = \sum_{|\psi_E\rangle} \left\langle \psi_E \left| \sum_j \mathbf{p}^+ \right| \varphi_j \right\rangle \langle \varphi_j|\mathbf{p}|\psi_E\rangle, \quad (1)$$

where $\varphi_j(\mathbf{r})=\varphi(\mathbf{r}-\mathbf{R}_j)$, $\mathbf{R}_j$ are the ionic positions, and where the sum is performed over the degeneracy of energy E. The scope of this work is to propose a method to compute quantities such as (1), and to test this method by calculating an electron-ion correlation function in liquid sodium.

The paper is organized as follows. We first propose that the one-electron expectation values $\langle \psi_E|A|\psi_E\rangle$ can be considered self-averaging quantities when $|\psi_E\rangle$ is delocalized. We then give a method to calculate $\langle \psi_E|A|\psi_E\rangle$ in the thermodynamic limit. We finally test the method by calculating an electron-ion correlation function in liquid sodium and by comparing our results with other methods.

II. SELF-AVERAGING PROPERTY IN THE DELOCALIZED REGIME

We consider a simple liquid or a plasma. It consists of N identical atoms contained in a box. Using a Born-Oppenheimer approximation, the ions have fixed positions in space and form a configuration, which has been effectively reached by the system. In the independent electron approximation, the electronic structure is dictated by a single electron Hamiltonian that includes both exchange and correlation effects. Using atomic units and denoting the Laplacian by Δ, we assume the Hamiltonian can be cast into the following form:

$$H=-\Delta/2+\sum_{j=1}^{N} V_j\,, \quad (2)$$

where $V_j(\mathbf{r})=V(\mathbf{r}-\mathbf{R}_j)$, with V a spherically symmetric operator and $\mathbf{R}_j$ an ionic position.

Assuming electrons are independent, and because the density of states is self-averaging, the thermodynamic average of an operator A is equal to the sum of averaged expectations over occupied one-electron eigenstates:

$$\mathrm{Tr}(\rho A)=\int f(E)n(E)\langle \mathrm{Tr}(\rho_E A)\rangle dE, \quad (3)$$

where f is the Fermi-Dirac occupation factor, n is the density of states, ρ_E is the projector at energy E, scaled by $\mathrm{Tr}(\rho_E)=1$, and where $\langle\ \rangle$ represents the average over configurations. To calculate $\langle \mathrm{Tr}(\rho_E A)\rangle$, we expand it as

$$\mathrm{Tr}(\rho_E A)=\int_{\mathbf{q}^2/2=E} \langle \psi_\mathbf{q}|A|\psi_\mathbf{q}\rangle d\hat{\mathbf{q}}/(4\pi q^2), \quad (4)$$

where $|\psi_\mathbf{q}\rangle$ is the general solution of Schrödinger's equation, as obtained from the exact Green's function (see [7], Chap. 4). Except for a normalization constant, it is

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$$|\psi_{\mathbf{q}}\rangle=\left(I+G_E^{\mathrm{Re}}\sum_{j=1}^{N}V_j\right)|\mathbf{q}\rangle, \tag{5}$$

where $|\mathbf{q}\rangle$ is a plane wave, $G_E^{\mathrm{Re}}=\mathrm{Re}(G_E^{+})=\frac{1}{2}(G_E^{+}+G_E^{-})$ is the real part of the Green's function related to H and $E=\mathbf{q}^2/2$. The wave function (5) does not satisfy the boundary conditions of the finite system. Hence it is not a proper solution for the problem considered. The trace, however, does not depend on a change of basis, so that (4) seems a reasonable approximation in a macroscopic system.

The central assumption in this work is that the one-electron expectation values of an operator A, which is symmetric with respect to exchange of ions, are self-averaging quantities when $|\psi_{\mathbf{q}}\rangle$ is delocalized. In the thermodynamic limit, $\langle\langle\psi_{\mathbf{q}}|A|\psi_{\mathbf{q}}\rangle\rangle=\langle\psi_{\mathbf{q}}|A|\psi_{\mathbf{q}}\rangle$ holds, and we have

$$\langle\mathrm{Tr}(\rho_E A)\rangle=\int_{\mathbf{q}^2/2=E}\langle\psi_{\mathbf{q}}|A|\psi_{\mathbf{q}}\rangle d\hat{\mathbf{q}}\Big/(4\pi q^2). \tag{6}$$

This applies to the expectation values of the identity and of the Hamiltonian (2). It also applies to the operator $A_{\mathbf{r}}(\mathbf{r}')=\Sigma_j\delta(\mathbf{r}'-\mathbf{R}_j-\mathbf{r})$ which yields the electron-ion correlation, and to the bound-free transition element given in Eq. (1).

Physically, this may be interpreted as follows. If a delocalized eigenstate is decomposed in localized orbitals, a change of ionic configuration caused by a local density fluctuation would affect only a small number of coefficients of the wave function. This, in turn, has an insignificant effect on the matrix element, which is a sum over all sites contributing to the extended wave function. In a macroscopic specimen, all local fluctuations can be considered present with a frequency proportional to their probability of occurrence. Local density fluctuations induce local changes in the coefficients, thus making the matrix element a sum over various local configurations. By contrast, this property does not hold in the localized regime. In this case, the expectation value obviously depends on the ionic configuration that exists in the region where the wave function takes nonzero values.

III. THE EXPECTATION VALUE

Because our goal is to propose a one-site approach, we decompose the extended wave function $|\psi_{\mathbf{q}}\rangle$ using a linear combination of atomic orbitals (LCAO)-like expansion. However, we allow the on-site ''basis'' $|\phi^n\rangle$ to be a finite set of nonorthogonal wave functions rather than atomic orbitals. Hence $|\psi_{\mathbf{q}}\rangle$ is expanded as

$$|\psi_{\mathbf{q}}\rangle=1\Big/\sqrt{N}\sum_{j,n}c_j^{\mathbf{q},n}|\phi_j^n\rangle, \tag{7}$$

where $\phi_j^n(\mathbf{r})=\phi^n(\mathbf{r}-\mathbf{R}_j)$, $c_j^{\mathbf{q},n}=\sqrt{N}\langle\overline{\phi_j^n}|\psi_{\mathbf{q}}\rangle$, and $\langle\overline{\phi_j^n}|$ are the conjugates of $|\phi_j^n\rangle$. Expression (7) can be expressed as

$$|\psi_{\mathbf{q}}\rangle=\sum_n|\psi_{\mathbf{q}}^n\rangle,\quad |\psi_{\mathbf{q}}^n\rangle=P_n|\psi_{\mathbf{q}}\rangle=\frac{1}{\sqrt{N}}\sum_j c_j^{\mathbf{q},n}|\phi_j^n\rangle, \tag{8}$$

where $P_n=\Sigma_j|\phi_j^n\rangle\langle\overline{\phi_j^n}|$. It is remarked that the states $(|\psi_{\mathbf{q}}^n\rangle)_{n\in[1,+\infty]}$ generate a space of wave functions that contains $|\psi_{\mathbf{q}}\rangle$ and make up a basis of this space. We propose to use these basis states to describe the state $|\psi_{\mathbf{q}}\rangle$. Interest in this basis arises from the matrix elements $\langle\psi_{\mathbf{q}}^n|A|\psi_{\mathbf{q}}^n\rangle=\langle\psi_{\mathbf{q}}|P_n^{+}AP_{n'}|\psi_{\mathbf{q}}\rangle$ being self-averaging quantities, as inferred from the hypothesis detailed in Sec. II. The matrix elements are

$$\begin{aligned}\langle\psi_q^{n'}|A|\psi_q^n\rangle&=\frac{1}{N}\sum_i\left\langle\sum_j c_i^{\mathbf{q},n}(c_j^{\mathbf{q},n'})^*\langle\phi_j^{n'}|A|\phi_i^n\rangle\right\rangle\\&=\langle(c_1^{\mathbf{q},n}(c_1^{\mathbf{q},n'})^*\langle\phi_1^{n'}|A|\phi_1^n\rangle\rangle\\&\quad+(N-1)\langle c_1^{\mathbf{q},n}(c_2^{\mathbf{q},n'})^*\langle\phi_2^{n'}|A|\phi_1^n\rangle\rangle.\end{aligned} \tag{9}$$

In this expression, terms such as $\langle\phi_2^{n'}|A|\phi_1^n\rangle$ are well-defined functions of the ionic configuration. Neglecting the correlation between the product $c_1^{\mathbf{q},n}(c_2^{\mathbf{q},n'})^*$ and the positions of the atoms different from 1 and 2, these matrix elements can be expressed in terms of correlation functions such as $u(\mathbf{R})=\langle c_1^{\mathbf{q},n}(c_2^{\mathbf{q},n'})^*\delta(\mathbf{R}-\mathbf{R}_1+\mathbf{R}_2)\rangle$. The problem of finding the matrix elements is thus transformed into that of finding these correlation functions. Neglecting the overlap integrals in the expression of the local projectors $|\phi_j^n\rangle\langle\overline{\phi_j^n}|$, the correlation functions are written as

$$u_{nn'}^{\mathbf{q}}(\mathbf{R})=\langle\langle\overline{\phi_2^n}|\psi_{\mathbf{q}}\rangle\langle\psi_{\mathbf{q}}|\overline{\phi_1^{n'}}\rangle\delta(\mathbf{R}-\mathbf{R}_1+\mathbf{R}_2)\rangle,$$

$$v_{nn'}^{\mathbf{q}}(\mathbf{R})=\langle\langle\overline{\phi_1^n}|\psi_{\mathbf{q}}\rangle\langle\psi_{\mathbf{q}}|\overline{\phi_1^{n'}}\rangle\delta(\mathbf{R}-\mathbf{R}_1+\mathbf{R}_2)\rangle.$$

Thus we essentially assume that the phase of $c_j^{\mathbf{q},n}$ is that of $|\psi_q\rangle$ at site $\mathbf{R}_j$. We finally approximate these correlation functions using the factorized form:

$$u_{nn'}^{q}(\mathbf{R})=\langle\overline{\phi^n}|\Phi_{\mathbf{q}}\rangle\xi^q(\mathbf{R})\langle\Phi_{\mathbf{q}}|\overline{\phi^{n'}}\rangle,$$

$$v_{nn'}^{q}(\mathbf{R})=\langle\overline{\phi^n}|\Phi_{\mathbf{q}}\rangle\xi^q(\mathbf{R})\langle\Phi_{\mathbf{q}}|\overline{\phi^{n'}}\rangle,$$

where $|\Phi_{\mathbf{q}}\rangle$, $\xi^{\mathbf{q}}(\mathbf{R})$, and $\zeta^{\mathbf{q}}(\mathbf{R})$ are to be determined.

Given trial functions $\xi^{\mathbf{q}}(\mathbf{R})$ and $\zeta^{\mathbf{q}}(\mathbf{R})$, $\Phi_{\mathbf{q}}$ may be obtained in the following way. If we scale the basis functions as $|\hat{\psi}_{\mathbf{q}}^n\rangle=|\psi_{\mathbf{q}}^n\rangle/\langle\overline{\phi^n}|\Phi_{\mathbf{q}}\rangle$, the correlation functions relevant to the calculation of $\langle\hat{\psi}_{\mathbf{q}}^n|A|\hat{\psi}_{\mathbf{q}}^{n'}\rangle$ are

$$\hat{u}_{nn'}^{\mathbf{q}}(\mathbf{R})=\frac{u_{nn'}^{\mathbf{q}}(\mathbf{R})}{\langle\overline{\phi^n}|\Phi_{\mathbf{q}}\rangle\langle\Phi_{\mathbf{q}}|\overline{\phi^{n'}}\rangle}=\xi^{\mathbf{q}}(\mathbf{R})$$

and similarly $\hat{v}_{nn'}^{\mathbf{q}}(\mathbf{R})=\zeta^{\mathbf{q}}(\mathbf{R})$. By using (9) we can calculate the matrix elements of the norm (which involves overlap integrals) and the Hamiltonian in the basis $|\hat{\psi}_{\mathbf{q}}^n\rangle$. The eigenvectors of the Hamiltonian are then obtained as combinations of the $|\hat{\psi}_{\mathbf{q}}^n\rangle$'s by (1) orthonormalizing the basis $|\hat{\psi}_{\mathbf{q}}^n\rangle$ with respect to the norm, which yields an orthonormal basis, and (2) diagonalizing the Hamiltonian in this new basis. Because $|\psi_{\mathbf{q}}\rangle$ belongs to the space generated by the $|\hat{\psi}_{\mathbf{q}}^{n}\rangle$'s it may be identified with the calculated eigenvector that has the eigenenergy closest to $E_{\mathbf{q}}=\mathbf{q}^2/2$. Thus, we obtain the coefficients of the expansion:

$$|\psi_{\mathbf{q}}\rangle=\sum_{n} a_{\mathbf{q}}^{n}|\hat{\psi}_{\mathbf{q}n}\rangle .$$

But since $|\psi_{\mathbf{q}}\rangle=\Sigma_n|\psi_{\mathbf{q}}^{n}\rangle$ [Eq. (8)], and because of $|\psi_{\mathbf{q}}^{n}\rangle=\langle\overline{\phi^n}|\Phi_{\mathbf{q}}\rangle|\hat{\psi}_{\mathbf{q}}^{n}\rangle$, then $a_{\mathbf{q}}^{n}=\langle\overline{\phi^n}|\Phi_{\mathbf{q}}\rangle$. This process therefore yields an approximation to $|\Phi_{\mathbf{q}}\rangle=\Sigma_n a_{\mathbf{q}}^{n}|\phi^n\rangle$.

The functions $\xi^{\mathbf{q}}(\mathbf{R})$ and $\zeta^{\mathbf{q}}(\mathbf{R})$ can be searched iteratively as the solutions of integral equations that we will present and use in a future publication. In the present paper, we only use the estimates that permit us to initiate the iterations. To zero order with respect to V expression (5) yields $\langle\langle\mathbf{R}_1|\psi_{\mathbf{q}}\rangle\langle\Psi_{\mathbf{q}}|\mathbf{R}_2\rangle\delta(\mathbf{R}-\mathbf{R}_1+\mathbf{R}_2)\rangle$ proportional to $e^{i\mathbf{q}\cdot r}$ Initial $\xi^{\mathbf{q}}(\mathbf{R})$ and $\xi^{\mathbf{q}}(\mathbf{R})$ are then obtained as

$$\xi^{\mathbf{q}}(\mathbf{R})=g(\mathbf{R})e^{i\mathbf{q}\cdot\mathbf{R}},\quad \xi^{\mathbf{q}}(\mathbf{R})=g(\mathbf{R}). \tag{10}$$

IV. APPLICATION

In this section, we use the method and the approximations described above to calculate an electron-ion correlation function $g_{e-i}(\mathbf{r})$ in liquid sodium, and we compare our results to (1) a calculation in crystalline bcc sodium, and (2) a calculation in which the site-to-site correlations are neglected.

The three calculations used the same screened pseudopotential [8,9]. The screening effect was computed in a bcc lattice adjusted to the liquid density ($\rho_0=0.928$ g/cm^3) by relaxing the electronic system using a Car-Parrinello code. The electron-ion correlation in crystalline bcc sodium was calculated in this process. The energy cutoff was 100 Ry. Exchange and correlation contributions were calculated using the local-density approximation (LDA). The transferability problems related to the nonlinearity of the LDA exchange correlation functional, which can be significant for the alkali-metal atoms, were taken care of following Louie *et al.* [10]. The isotropy of the resulting potential was good.

This screened pseudopotential is then placed in a uniform electronic density ρ_0, and the displaced charge $\delta\rho(\mathbf{r})=\rho(\mathbf{r})-\rho_0$ is calculated by solving the partial spherical waves. The electron-ion correlation function is then obtained within the charge superposition approximation by convolution with the ion-ion correlation function $g(\mathbf{r})$ (a hard-sphere model [11] and a hard-sphere packing fraction equal to $\eta=0.433$ [12] were used). This method of calculation, which consists of a superposition of independently displaced charges (SIDC), neglects the electronic correlations from site to site and is quite close to linear response theory (see [13], for instance).

By contrast, the displaced charge calculated with our method accounts for the existence of neighbors. Denoting $A_{\mathbf{r}}(\mathbf{r}')=\Sigma_j\delta(\mathbf{r}'-\mathbf{R}_j-\mathbf{r})$, the electron-ion correlation is equal to

$$\rho_0 g_{e-i}(\mathbf{r})=\sum_{\mathbf{q}} f(E_{\mathbf{q}})n(E_{\mathbf{q}})\langle\psi_{\mathbf{q}}|A_{\mathbf{r}}|\psi_{\mathbf{q}}\rangle,$$

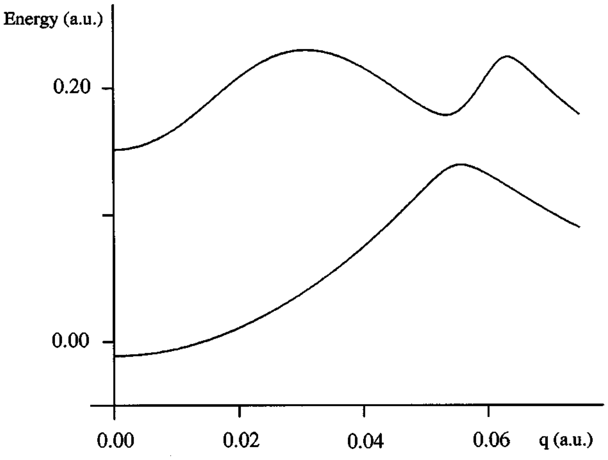

FIG. 1. Calculated energies for liquid sodium: the lowest two eigenenergies (in atomic units).

where $\langle\psi_{\mathbf{q}}|A_{\mathbf{r}}|\psi_{\mathbf{q}}\rangle=\Sigma_{nn'}a_{\mathbf{q}}^{n*}a_{\mathbf{q}}^{n'}\langle\hat{\psi}_{\mathbf{q}}^{n}|A_{\mathbf{r}}|\psi_{\mathbf{q}}^{n'}\rangle$ is calculated by using a small basis set of atomic orbitals (the $3s$, $3p$, $3d$, and $4s$ states denoted $|\phi^n\rangle$). Figure 1 shows the two lowest calculated eigenvalues. The self-consistency condition $E=q^2/2$ is well satisfied up to $\mathbf{q}\approx0.5$ a.u., but the basis set we used is too small to accurately describe higher energies. However, since the Fermi level is reached for $\mathbf{q}\approx0.47$ a.u., our calculation can be used to obtain the electron-ion correlation function. Using a free-electron density of states, this is decomposed as

$$\begin{aligned}\rho_0 g_{e-i}(\mathbf{r})=\sum_{n,n'}\Bigg\{&\phi^n(\mathbf{r})^*\phi^{n'}(\mathbf{r})\int_{|q|<k_F} d\mathbf{q}a_{\mathbf{q}}^{n*}a_{\mathbf{q}}^{n'}\\ &+\rho_0\int d\mathbf{R}g(\mathbf{R})[\phi^n(\mathbf{r})^*\phi^{n'}(\mathbf{r}-\mathbf{R})\\ &+\phi^n(\mathbf{r}+\mathbf{R})^*\phi^{n'}(\mathbf{r})]\int_{|\mathbf{q}|<k_F} d\mathbf{q}a_{\mathbf{q}}^{n*}a_{\mathbf{q}}^{n'}e^{i\mathbf{q}\cdot\mathbf{R}}\\ &+\rho_0\int d\mathbf{R})g(\mathbf{R})\phi^n(\mathbf{r}+\mathbf{R})^*\phi^{n'}(\mathbf{r}+\mathbf{R})\\ &\times\int_{|q|<k_F} d\mathbf{q}a_{\mathbf{q}}^{n*}a_{\mathbf{q}}^{n'}+\rho_0^2\int d\mathbf{R}_1 d\mathbf{R}_2 n^3(0,\mathbf{R}_1,\mathbf{R}_2)\\ &\times\phi^n(\mathbf{r}+\mathbf{R}_2)^*\phi^{n'}(\mathbf{r}+\mathbf{R}_2-\mathbf{R}_1)\\ &\times\int_{|\mathbf{q}|<k_F} d\mathbf{q}a_{\mathbf{q}}^{n*}a_{\mathbf{q}}^{n'}e^{i\mathbf{q}\cdot\mathbf{R}_1}\Bigg\}.\end{aligned} \tag{11}$$

The four terms that appear in (11) may be interpreted as (a) the charge that follows an ion, (b) the bonds between an ion and its neighbors, (c) the charge that follows its neighbors, and (d) the bonds between its neighbors. The charge superposition approximation is obtained by neglecting some correlations in the fourth sum. The charge $\widetilde{\rho}$ associated with each ion is then the sum of the charge that follows an ion (a) with half the charge of the bond (b). Using the same $g(\mathbf{r})$ that was used in the SIDC, the resulting electron-ion correlation function is

$$\rho_0 g_{e-i}(\mathbf{r}) = \widetilde{\rho}(\mathbf{r}) + \rho_0 \int d\mathbf{r}' g(\mathbf{r}') \widetilde{\rho}(\mathbf{r}-\mathbf{r}').$$

Results are shown in Fig. 2. As expected, the SIDC results are similar to those obtained in Ref. [13]. They show the same positions for the peaks and problems of negative density for small radii. The results obtained using the new method differ significantly from these for radii smaller than 10 a.u.. The first peak is displaced (2.8 a.u. for the new method instead of 3.2). The problems of negative density for small radii, found with SIDC, have disappeared. Furthermore, the agreement between the new density and the one obtained from the electronic minimization in bcc sodium is good.

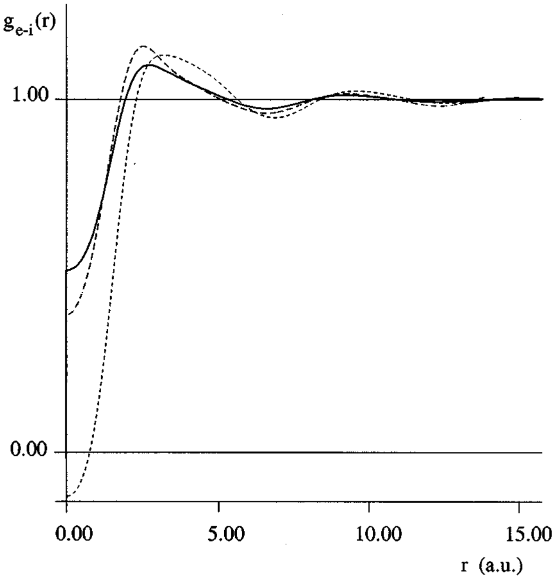

FIG. 2. Electron-ion correlation functions in liquid sodium. The dotted line is the superposition of independently displaced charges (SIDC). The dashed line is the electronic minimization in a bcc crystal. The heavy line corresponds to the proposed method.

V. CONCLUSIONS

Assuming that expectations $\langle \psi_{\mathbf{q}} | A | \psi_{\mathbf{q}} \rangle$ are self-averaging if $|\psi_{\mathbf{q}}\rangle$ is delocalized, we express the expectation value in terms of some correlation functions. Hence, the expectation value of an operator $\mathrm{Tr}(\rho A)$ may be calculated in terms of (1) the density of states, and (2) the correlation functions. A scheme to get approximate correlation functions is then proposed, and a numerical application is performed in the case of liquid sodium: the electron-ion correlation function is computed and assessed. Future work includes development of a self-consistent one-center potential [i.e, $V(\mathbf{r})$ in Eq. (2)] that is consistent with a given ionic disorder, and calculation of the photoelectric effect.

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