Dielectric Formulation for Many-Particle Systems with General Interactions*

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An extension of the self-consistent field approach formulation by Cohen in the preceding paper is proposed in order to include the most general kind of two-body interactions, i.e., interactions depending on position, momenta, spin, isotopic spin, etc. The dielectric function is replaced by a dielectric matrix. The evaluation of the energies involves the computation of a matrix inversion and trace.

IN this note we propose a further extension of the self-consistent field (SCF) approach formulated by Cohen,[1] in order to include the most general kind of two-body interactions. We formulate the problem in the second-quantization formalism and derive a formula for the energy similar to (III.21) of reference 1 in which the dielectric function is replaced by a dielectric matrix. The fundamental parameter ξ has here the same meaning and properties.

The system to be considered is that of N particles of one species; the Hamiltonian is given by

$$\mathcal{H}(g)=\int \psi^\dagger(x)\left[-\frac{\hbar^2}{2m}\nabla^2+U(x)\right]\psi(x)dx +\tfrac{1}{2}\int\int \psi^\dagger(x)\psi^\dagger(x')v(g;x,x',\nabla_x,\nabla_{x'}) \times\psi(x')\psi(x)dxdx', \quad (1)$$

where g is the strength of the interaction and x denotes the spatial coordinates as well as spin, isotopic spin, etc. In general, v depends on g in an arbitrary fashion and is a function of coordinates and momenta. Suitable limiting procedures depending on g allow the treatment of highly singular interactions. By introducing a complete set of functions φ_n in the x space and the corresponding creation and destruction operators $a_n^\dagger$ and a_n,

$$\psi(x)=\sum\nolimits_n \varphi_n(x)a_n, \quad (2)$$

$$\mathcal{H}(g)=\sum\nolimits_{nm} K_{nm}a_n^\dagger a_m+\tfrac{1}{2}\sum\nolimits_{nmrs} v_{ns,rm}a_n^\dagger a_m^\dagger a_r a_s, \quad (3)$$

where

$$K_{nm}=\int \varphi_n^\dagger(x)\left[-\frac{\hbar^2}{2m}\nabla^2+U(x)\right]\varphi_m(x)dx, \quad (4)$$

$$v_{ns,rm}=\int\int \varphi_n^\dagger(x)\varphi_m^\dagger(x') \times v(g;x,x',\nabla_x,\nabla_{x'})\varphi_r(x')\varphi_s(x)dxdx'. \quad (5)$$

The energy of the ground state is obtained by minimizing with respect to $|0,g,1\rangle$ the expression

$$E_0(g,1)=\langle 0,g,1|\mathcal{H}(g)|0,g,1\rangle. \quad (6)$$

The SCF formulation, in zeroth order, is obtained when the definition of the energy $E_0(g,1)$ is replaced by

$$E_0(g,0)=\sum\nolimits_{nm} K_{nm}\langle 0,g,0|a_n^\dagger a_m|0,g,0\rangle +\tfrac{1}{2}\sum\nolimits_{nmrs} v_{ns,rm}\langle 0,g,0|a_n^\dagger a_s|0,g,0\rangle \times\langle 0,g,0|a_m^\dagger a_r|0,g,0\rangle. \quad (7)$$

This immediately yields

$$\mathcal{H}(g,0)|0,g,0\rangle=\mathcal{E}_{00}|0,g,0\rangle, \quad (8)$$

where

$$\mathcal{H}(g,0)=\sum_{mr}[K_{mr}+V_{mr}(0)]a_m^\dagger a_r, \quad (9)$$

$$V_{mr}(0)=\tfrac{1}{2}\sum_{ns}(v_{ns,rm}+v_{mr,sn})\langle 0,g,0|a_n^\dagger a_s|0,g,0\rangle, \quad (10)$$

$$E_0(g,0)=\mathcal{E}_{00}-\tfrac{1}{2}\sum_{mr}V_{mr}(0)\langle 0,g,0|a_m^\dagger a_r|0,g,0\rangle. \quad (11)$$

Following reference (1) we now introduce the parameter ξ to obtain the generalized SCF formulation,

$$E_0(g,\xi)=\sum_{mr}K_{mr}\langle 0,g,\xi|a_m^\dagger a_r|0,g,\xi\rangle +\frac{1-\xi}{2}\sum_{mnrs}v_{ns,rm}\langle 0,g,\xi|a_n^\dagger a_s|0,g,\xi\rangle \times\langle 0,g,\xi|a_m^\dagger a_r|0,g,\xi\rangle +\frac{\xi}{2}\sum_{mnrs}v_{ns,rm}\langle 0,g,\xi|a_n^\dagger a_m^\dagger a_r a_s|0,g,\xi\rangle, \quad (12)$$

such that the energy reduces to (7) at $\xi=0$ and to the exact case (6) at $\xi=1$.

Variation of (12) with respect to the state vector gives

$$\mathcal{H}(g,\xi)|0,g,\xi\rangle=\mathcal{E}_{0\xi}|0,g,\xi\rangle, \quad (13)$$

$$\mathcal{H}(g,\xi)=\sum_{mr}[K_{mr}+(1-\xi)V_{mr}(\xi)]a_m^\dagger a_r +\frac{\xi}{2}\sum_{mnrs}v_{ns,rm}a_n^\dagger a_m^\dagger a_r a_s, \quad (14)$$

where $V_{mr}(\xi)$ is given by (10) with the state vector $|0,g,\xi\rangle$ instead of $|0,g,0\rangle$ and

$$E_0(g,\xi)=\mathcal{E}_{0\xi}-\tfrac{1}{2}\sum_{mr}V_{mr}(\xi)\langle 0,g,\xi|a_m^\dagger a_n|0,g,\xi\rangle. \quad (15)$$

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[1] M. H. Cohen, Phys. Rev. 130, 1301 (1963).

From now on it is possible to follow step by step the derivation of reference 1 with parallel results. So by computing $dE_0/d\xi$ the energy $E_0(g,\xi)$ can be expressed

$$E_0(g,\xi)=E_0(g,0)+\frac{1}{4}\int_0^\xi d\xi \sum_\alpha{}' \sum_{nmrs} [v_{ns,rm}+v_{mr,sn}] \times\langle 0,g,\xi|a_n^\dagger a_s|\alpha,g,\xi\rangle\langle\alpha,g,\xi|a_m^\dagger a_r|0,g,\xi\rangle, \quad (16)$$

where $|\alpha,g,\xi\rangle$ is a general eigenstate of (14) and the sum excludes the term with $\alpha=0$.

Similarly, by extending the formulation to time-dependent problems, we get a Schrödinger equation

$$i\hbar|\dot{x}\rangle=\mathcal{H}(x)|x\rangle, \quad (17)$$

where $\mathcal{H}(x)$ is given by (14) but with $V_{mr}(\xi)$ replaced by

$$V_{mr}(x)=\tfrac{1}{2}\sum_{ns}[v_{ns,rm}+v_{mr,sn}]\langle x|a_n^\dagger a_s|x\rangle. \quad (18)$$

The introduction of a time-dependent perturbation

$$\mathcal{H}_1=\sum_{rs}A_{rs}a_r^\dagger a_s, \qquad A_{rs}\propto e^{i\omega t}e^{\delta t}, \quad \delta\to 0^+, \quad (19)$$

produces a response in the system characterized by a dielectric matrix, i.e., the effective perturbation felt by a test particle is given by

$$A_{rs}'=\sum_{mn}(\boldsymbol{\varepsilon}^{-1})_{rs,mn}A_{mn}, \quad (20)$$

where $\boldsymbol{\varepsilon}^{-1}$ is the inverse dielectric matrix. The dielectric matrix is defined as

$$\boldsymbol{\varepsilon}=\mathbf{I}-(\boldsymbol{v}\cdot\boldsymbol{\mathfrak{D}})[\mathbf{I}+\xi\boldsymbol{v}\cdot\boldsymbol{\mathfrak{D}}]^{-1}, \quad (21)$$

where $\mathbf{I}$ is the unit matrix of elements

$$I_{mn,rs}=\delta_{mr}\delta_{ns}. \quad (22)$$

$\boldsymbol{v}$ is the interaction matrix whose elements are given by (5), and

$$\mathfrak{D}_{mn,rs}(\omega,\xi)=\sum_\alpha{}'\left[\frac{\langle 0,g,\xi|a_n^\dagger a_m|\alpha,g,\xi\rangle\langle\alpha,g,\xi|a_r^\dagger a_s|0,g,\xi\rangle}{-\hbar\omega-\mathcal{E}_{\alpha\xi}+\mathcal{E}_{0\xi}+i\delta}+\frac{\langle 0,g,\xi|a_r^\dagger a_s|\alpha,g,\xi\rangle\langle\alpha,g,\xi|a_n^\dagger a_m|0,g,\xi\rangle}{\hbar\omega-\mathcal{E}_{\alpha\xi}+\mathcal{E}_{0\xi}-i\delta}\right]. \quad (23)$$

From (21), (23), and (16) we find

$$E_0(g,1)=E_0(g,0)-\frac{\hbar}{2\pi}\int_0^1 d\xi\int_0^\infty d\omega\ \mathrm{Im}\left\{\mathrm{Tr}\left[\frac{\boldsymbol{\varepsilon}-\mathbf{I}}{\mathbf{I}+\xi(\boldsymbol{\varepsilon}-\mathbf{I})}\right]\right\}. \quad (24)$$

It is easily shown that for the uniform spinless case in the momentum representation

$$\mathfrak{D}_{mn,rs}=\delta_{n+r,m+s}\mathfrak{D}_{mn,rs}, \qquad v_{rs,mn}=v(|r-s|)\delta_{n+r,m+s}. \quad (25)$$

Using (21), we have

$$\mathrm{Im}\left\{\mathrm{Tr}\left[\frac{\boldsymbol{\varepsilon}-\mathbf{I}}{\mathbf{I}+\xi(\boldsymbol{\varepsilon}-\mathbf{I})}\right]\right\}=-\sum_q v(q)\ \mathrm{Im}\mathfrak{D}_q(\omega), \quad (26)$$

where

$$\mathfrak{D}_q(\omega)=\sum_{mr}\mathfrak{D}_{m\ m+q,r\ r-q}. \quad (27)$$

If (26) is substituted in (24), formula (II.47) of reference (1) is obtained.

For general systems the evaluation of (24) involves the calculation of a very complicated matrix inversion and a trace, and the matrix is in general of infinite order. For uniform cases the infinite trace can be reduced to a finite one, i.e., to the order of the dimensions of the combined space of spin and isotopic spin, and integration over momenta.

Finally for hard-core interactions, a suitable limiting procedure on the g's may give reasonable results if enough care is exercised in varying the two parameters g and ξ. This may result in velocity-dependent potentials when the hard-core regions are excluded. An application of these techniques may give interesting results in the case of nuclear matter and liquid helium.

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