Theory of Perturbations with a Strong Interaction

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Abstract

The theory of perturbations is suggested for statistical systems in the absence of small interaction parameters. A new form is advanced for self-consistent conditions defining the optimal parameters for trial Green functions in iterating nonlinear propagator equations. Superharmonic, semiharmonic, and pseudoharmonic approximations for a molecular crystal are considered as examples.

Theory of Perturbations

Let us consider a statistical system in the five-dimensional space \( \{ y \} \).

\[
y = \{ x, t \}; \quad x = \{ r, f \}; \quad r = \{ r_i \}; \quad i = 1, 2, 3,
\]

where \( f \) is a variable characterizing internal degrees of freedom or macroscopic state indices \( [1, 2] \) (or their combination). For brevity, we shall write

\[
\varphi(y_1 \ldots y_n) \equiv \varphi(1 \ldots n); \quad dy_1 \ldots dy_n \equiv d(1 \ldots n).
\]  

(1)

We assume that the exact solution of the equation of motion

\[
\int G^{-1}(13) G(32) d(3) = \delta(12)
\]

is unknown, but the solution of some model problem

\[
\int G_0^{-1}(13) G_0(32) d(3) = \delta(12)
\]

(3)
can be found. Here and subsequently $G$ denotes a causal Green’s function, which is defined in the usual manner through field operators, or axiomatically [3]. Introducing the kernel

\[ K(12) = \int G_0(13) \left[ G^{-1}_0(32) - G^{-1}(32) \right] d(3), \]  

we can write, on the basis of (2) and (3), the Dyson equation

\[ G(12) = G_0(12) + \int K(13)G(32)\,d(3). \]  

The nonlinear integral equation (5) can be solved by some approximate methods [4]. We shall, for example, integrate it following the scheme

\[ G_n \rightarrow K_{n+1} \rightarrow G_{n+1}, \]

in which $K_n$ is the $n$-iterated functional (4),

\[ K_{n+1} \equiv K\{G_{n+1}^{-1}\}, \quad G_{n+1}^{-1} \equiv G^{-1}\{G_n\}. \]

Obviously, if the particle interaction is sufficiently strong, then the propagator of free particles cannot be taken as a zero approximation. One should take as $G_0$ a trial Green function, whose parameters are to be defined from additional conditions. The following self-consistent optimal conditions are suggested: the average values of some operators $\mathcal{O}$, corresponding to observable quantities, calculated in the $n + 1$-th and $n$-th iterations coincide, i.e.,

\[ \int \lim_{x_2 \to x_1} \lim_{t_{12} \to -0} \mathcal{O}(1)[G_{n+1}(12) - G_n(12)]\,dx_1 = 0. \]  

The expression $t_{12}$ implies the difference $t_1 - t_2$. It is necessary to take as many different equalities (6) as there is the number of trial parameters contained in $G_0$. Of all possible operators, one should select those $\mathcal{O}$, the averages of which have to be known with the greatest accuracy in the given problem. When the left-hand side of (6) is proportional to the average number or particles, then in taking thermodynamic limit one should divide Eq. (6) by

\[ N = \pm i \int \lim_{x_2 \to x_1} \lim_{t_{12} \to -0} G(12)\,dx_1. \]

Stopping at the first iteration step and making use of (5), we get, instead of (6),

\[ \int \lim_{x_2 \to x_1} \lim_{t_{12} \to -0} \mathcal{O}(1)K_1(13)G_0(32)\,d(3)\,dx_1 = 0. \]  

Condition (7) can be employed for both equilibrium and nonequilibrium systems. In the case of the former it is better to use Fourier representation with respect to $\tau \equiv t - t'$,

\[ \varphi(y, y') = \frac{1}{2\pi} \int \varphi(x, x', \omega)e^{-i\omega\tau}\,d\omega, \]

where the definite integral over the interval $(-\infty, +\infty)$ is assumed. Here

\[ K(x, x', \omega) = \int G_0(x, x'', \omega)\left[ G^{-1}_0(x'', x', \omega) - G^{-1}(x'', x', \omega) \right]\,dx'', \]
\[ N = \pm \frac{i}{2\pi} \int \lim_{x' \to x} \lim_{\tau \to +0} G(x, x', \omega) e^{i\omega \tau} d\omega dx, \]

while Eq. (7) becomes
\[
\lim_{\tau \to +0} \int G_0(x', x, \omega) \mathcal{O}(x) K_1(x, x', \omega) e^{i\omega \tau} d\omega dx dx' = 0 .
\]

The operator \( \mathcal{O}(x) \) is the same as \( \mathcal{O}(y) \).

**Self-Consistent Conditions**

Let us see how the self-consistent conditions (8) are simplified in certain particular cases. Let \( G \) be expanded in wave functions
\[
G_0(x, x') = \sum_n G_n(\omega) \psi_n(x) \psi_n^*(x') .
\]

The subscript \( n \) in this expression means the total set of quantum indices characterizing the wave functions. In what follows, the upper sign is to be taken for Bose systems and the lower sign is to be used for Fermi systems:
\[
G_n(\omega) = \frac{1 \pm n(\omega_n)}{\omega - \omega_n + i0} \mp \frac{n(\omega_n)}{\omega - \omega_n - i0} ,
\]

\[
n(\omega) = (\exp(\beta \omega) \mp 1)^{-1} .
\]

Using the notations
\[
\Delta(x, x', \omega) = G_0^{-1}(x, x', \omega) - G_1^{-1}(x, x', \omega) ,
\]
\[
\Delta_{mn}(\omega) = \int \psi_m^*(x) \Delta(x, x', \omega) \psi_n(x') dxdx' ,
\]
\[
\mathcal{O}_{mn} = \int \psi_m^*(x) \mathcal{O}(x) \psi_n(x) dx ,
\]
we transform Eq. (8) to
\[
\lim_{\tau \to +0} \int e^{i\omega \tau} \sum_{mn} G_m(\omega) G_n(\omega) \mathcal{O}_{mn} \Delta_{mn}(\omega) d\omega = 0 .
\]

Now \( N = \sum_n n(\omega_n) \). In converting from (8) to (11) it must be remembered that
\[
\lim_{x' \to x} G(x, x', \omega) = \pm \lim_{x' \to x} G(x', x, -\omega) .
\]

We assume that \( \Delta(x, x', \omega) \) is not a function of frequency \( \omega \),
\[
\Delta(x, x', \omega) = \Delta(x, x') ,
\]
consequently, also \( \Delta_{mn}(\omega) \equiv \Delta_{mn} \) is not a function of \( \omega \). Noting that
\[
\lim_{\tau \to +0} \int e^{i\omega \tau} G_m(\omega) G_n(\omega) d\omega = \pm 2\pi i \frac{n(\omega_m) - n(\omega_n)}{\omega_n - \omega_m} ,
\]
we find from (11)

\[
\sum_{mn} O_{mn} \frac{n(\omega_m) - n(\omega_n)}{\omega_n - \omega_m} \Delta_{nm} = 0 .
\]  

(13)

If we assume that eigenfunctions of operator \( O(x) \) coincide with \( \psi_n(x) \)

\[
O(x) \psi_n(x) = O_n \psi_n(x) ,
\]

then \( O_{mn} = \delta_{mn} O_n \), and since

\[
\lim_{m \to n} \frac{n(\omega_m) - n(\omega_n)}{\omega_n - \omega_m} = \beta n^2(\omega_n) e^{\beta \omega_n} ,
\]

equation (13) reduces to

\[
\sum_n O_n n^2(\omega_n) e^{\beta \omega_n} \Delta_{nn} = 0 .
\]  

(14)

It should be noted that the limiting transitions \( m \to n \), \( \tau \to +0 \) for the integral

\[
I_{mn}(\tau) = \int e^{i\omega \tau} G_m(\omega) G_n(\omega) \, d\omega
\]

are noncommutative:

\[
\lim_{m \to n} \lim_{\tau \to +0} I_{mn}(\tau) = \pm 2\pi i n^2(\omega_n) e^{\beta \omega_n} , \quad \lim_{\tau \to +0} \lim_{m \to n} I_{mn}(\tau) = \mp \infty .
\]

Only the first sequence of limits is meaningful, which is natural, since initially one specifies the equation of motion, also fixing \( \Delta(x, x', \omega) \), and only then the operators \( O(x) \) are selected for self-consistent conditions.

Here it is particularly important to use causal Green functions. When (12) applies, Eq. (11) for retarded Green functions becomes an identity due to the fact that for then \( \lim_{\tau \to +0} I_{mn}(\tau) \equiv 0 \).

If \( n(\omega_n) \) decreases rapidly with the increase in \( n \), then it is possible to retain a finite number of terms in summation (14). Retaining the first term with \( n = 0 \), we obtain the self-consistent condition

\[
\int \psi_0^*(x) \Delta(x, x') \psi_0(x') \, dx \, dx' = 0 .
\]  

(15)

Example of Application

Let us consider the application of the suggested techniques for an example of a nonmagnetic localized crystal, for which the Green’s function is represented as a sum over the lattice sites \( G = \sum G_a \), and when a pseudo-Hartree (Hartree approximation with an effective potential) equations \([5,6]\) can be used. A classical crystal in the Hartree approximation has been treated in \([7]\).

In the considered case, Eq. (10) becomes

\[
\Delta(r, r', \omega) = [V_1(r) - V_0(r)] \delta(r - r') .
\]
The average field
\[ V_1(\mathbf{r}) = \int \rho(\mathbf{r}') \sum_a \Phi(\mathbf{r}, \mathbf{r}' + \mathbf{a}) \, d\mathbf{r}', \]
where \( \mathbf{a} \) is a lattice vector and \( \Phi \) is a pseudopotential taking into account pair particle correlations. As is known [8], taking for \( \Phi \) an interaction potential of bare particles most frequently produces divergences.

For a zero approximation, we can accept the potential of the isotropic harmonic oscillator
\[ V_0(\mathbf{r}) = u_0 + \frac{m_0 \omega_0^2}{2} (\mathbf{r} - \mathbf{a})^2 ; \quad u_0 = w \sum_b \Phi(\mathbf{a}, \mathbf{b}). \]

Here \( w \) is the number of particles per elementary cell:
\[ w = \int \rho(\mathbf{r}) \, d\mathbf{r} = \sum_{nml} n(\omega_{nl}) , \quad \rho(\mathbf{r}) = \sum_{nml} n(\omega_{nl})|\psi_{nml}(\mathbf{r})|^2 , \]
\[ \omega_{nl} = u_0 + \omega_0 \left( 2n + l + \frac{3}{2} \right) - \mu. \]

An anharmonic oscillator [9,10] could be taken for a starting approximation, however, this would have rapidly resulted in unjustified complication of calculations and hence it is unreasonable.

To describe the single trial parameter \( \omega_0 \) we shall use the self-consistency condition (14) with the unit operator \( \mathcal{O} \):
\[ \sum_{nml} n^2(\omega_{nl}) e^{\beta \omega_{nl}} \Delta_{nml} = 0 , \]  
\[ \Delta_{nml} = \int |\psi_{nml}(\mathbf{r} - \mathbf{a})|^2 \left[ V_1(\mathbf{r}) - V_0(\mathbf{r}) \right] d\mathbf{r} . \]  

The average
\[ \langle \varphi(\mathbf{r}) \rangle_{nm} = \int |\psi_{nml}(\mathbf{r})|^2 \varphi(\mathbf{r}) \, d\mathbf{r} \]
for \( \varphi = r^2 \) can be easily found from the virial theorem, which yields
\[ \langle r^2 \rangle_{nml} = \left( 2n + l + \frac{3}{2} \right) \frac{1}{m_0 \omega_0} . \]

Since \( n(\omega_{nl}) \) falls off rapidly with increasing \( n \) and \( l \), it is possible to retain a single term from (16) with \( n = l = 0 \), which is equivalent to (15). Then We find for \( \omega_0 \)
\[ \omega_0 = \frac{4}{3} (\Phi_0 - u_0) , \quad \Phi_s = w \sum_{b} |\psi_0(\mathbf{r})|^2 |\psi_0(\mathbf{r}')|^2 \Phi(\mathbf{r} + \mathbf{a}, \mathbf{r}' + \mathbf{b}) \, d\mathbf{r} d\mathbf{r}', \]
where
\[ w = n(E_0 - \mu) , \quad E_0 = u_0 + \frac{3 \omega_0}{2} . \]

As far as the trial frequency \( \omega_0 \) is defined through the total potential \( \Phi \), without involving its expansion in Taylor series, that is, with allowance for the anharmonicity of all orders, without
exception, this approximation can be termed superharmonic. Usually, however, the interaction potential is expanded in series in terms of the deviations from the lattice sites.

The principal contribution to integral (17) is made by the region near \( \mathbf{r} = \mathbf{a} \), and it is hence sensible to use the expansion

\[
\Phi(\mathbf{r} + \mathbf{a}, \mathbf{r'} + \mathbf{b}) = \sum_{n=0}^{\infty} \frac{1}{n!} \partial_{ab}^n(\mathbf{r}, 0) \Phi(\mathbf{a}, \mathbf{r'} + \mathbf{b}),
\]

\[
\partial_{ab}(\mathbf{r}, \mathbf{r'}) = \sum_{i=1}^{3} \left( r_i \frac{\partial}{\partial a_i} + r'_i \frac{\partial}{\partial b_i} \right).
\]  

(18)

Using the second order of the above expansion and employing to the properties

\[
\int r_i \rho(\mathbf{r}) \, d\mathbf{r} = 0, \quad \int r_i r_j \rho(\mathbf{r}) \, d\mathbf{r} = \delta_{ij} \int r_i^2 \rho(\mathbf{r}) \, d\mathbf{r},
\]

\[
\sum_{m=-l}^{+l} \langle r_i^2 \rangle_{nlm} = \frac{1}{3} \langle r^2 \rangle_{nlm},
\]

and the notation

\[
\Phi_h = w \sum_a \langle \Phi(\mathbf{a}, \mathbf{r} + \mathbf{b}) \rangle_0, \quad \omega_1^2 = w \sum_a \sum_{i=1}^{3} \frac{\partial^2}{\partial a_i^2} \langle \Phi(\mathbf{a}, \mathbf{r} + \mathbf{b}) \rangle_0,
\]

we find from (15) the trial frequency

\[
\omega_0 = \frac{1}{3} \left| 2(\Phi_h - u_0) + \sqrt{4(\Phi_h - u_0)^2 + 9\omega_h^2} \right|
\]

as the frequency in the semiharmonic approximation. Retaining the \( n + 1 \) terms in expansion (18), we would have obtained an \( n-th \) order semiharmonic approximation.

If we carry out expansion (17) with the consideration of the fact that the function \( \psi_{nlm}(\mathbf{r} - \mathbf{a}) \) decreases fast with the distance from the lattice site \( \mathbf{r} = \mathbf{a} \), and expand the pseudopotential, then expanding it in both coordinates, we get

\[
\Phi(\mathbf{r} + \mathbf{a}, \mathbf{r'} + \mathbf{b}) = \sum_{n=0}^{\infty} \frac{1}{n!} \partial_{ab}^n \Phi(\mathbf{a}, \mathbf{b}).
\]  

(19)

We introduce the notation

\[
\omega_1^2 = \frac{w}{3m_0} \sum_b \sum_{i=1}^{3} \frac{\partial^2}{\partial a_i^2} \Phi(\mathbf{a}, \mathbf{b}), \quad \omega_2^2 = \frac{w}{3m_0} \sum_b \sum_{i=1}^{3} \frac{\partial^2}{\partial b_i^2} \Phi(\mathbf{a}, \mathbf{b}),
\]

\[
r_0^2 = \frac{1}{w} \sum_{nl} n(\omega_{nl}) \langle r^2 \rangle_{nlm}.
\]

Equation (16) in the second order of expansion (19) contains the quantity

\[
\frac{2}{m_0} \sum_{nl} \Delta_{nlm} = \left[ \omega_1^2 + (2l + 1)\omega_0^2 \right] \langle r^2 \rangle_{nlm} + (2l + 1)\omega_2^2 r_0^2.
\]
This approximation, which is identical to the pseudoharmonic in the simplest case of \( n = l = 0 \), when
\[
\langle r^2 \rangle_0 = \frac{3}{2m_0} \omega_0 ,
\]
yields
\[
\omega_0 = \sqrt{\omega_1^2 + \omega_2^2} .
\] (20)

Incorporating \( n + 1 \) terms in (19) would have resulted in an \( n \)-th order pseudoharmonic approximation.

For the potential \( \Phi(r, r') = \Phi(r - r') \), since \( \omega_1 = \omega_2 \), then on the basis of (20), we would have \( \omega_0 = \omega_1 \sqrt{2} \).

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