

A METHOD OF GREEN FUNCTION DECOUPLING

BY K. PARLIŃSKI

Institute of Nuclear Physics, Cracow*

(Received September 12, 1970)

A method of approximation of spectral density function by a set of δ -functions is given. The one δ -function approximation corresponds to the introduction of the noninteracting quasi-particles system. This method, based on the classical problem of moments is equivalent to a certain retarded Green function decoupling procedure.

The retarded Green's function method has been widely used in the study of equilibrium properties of an interacting many-body system [1]. One of the approximation procedures used for simplifying Green function calculation is that of equation of motion decoupling. This procedure always gives reasonable results. The retarded Green function method permits the fluctuation in the system to be found, but does not give the energy of the ground state.

In this paper we propose a new technique, equivalent to some known decoupling procedures, which is based on the classical problem of moments [2]. The retarded Green function is approximated here by the frequency moments of the spectral density function. The spectral density function is obtained as a set of δ -functions, the number of which increases when the order of the approximation increases. The single δ -function approach is equivalent to the introduction of a non-interacting quasiparticles system. Unfortunately, the life-time of quasi-particles cannot be found at present.

1. Let the system be given by the Hamiltonian H . We introduce the commutator correlation function

$$\langle [A(t), B(t')]_{\eta} \rangle \quad (1)$$

where $A(t), B(t')$ are operators in Heisenberg representation, and the parameter $\eta = +1$ (commutator) or $\eta = -1$ (anticommutator) is chosen for convenience. The latter is independent of the commutator relation of A and B operators.

The spectral density function $K(\omega)$ is a Fourier transform of the commutator correlation function,

$$K(\omega) = \int_{-\infty}^{\infty} dt \langle [A(t), B(0)]_{\eta} \rangle e^{i\omega t} \quad (2)$$

* Address: Instytut Fizyki Jądrowej, Kraków 23 (Bronowice), Radzikowskiego 152, Poland.

$$\langle [A(t), B(t')]_{\eta} \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega K(\omega) e^{-i\omega(t-t')}. \quad (3)$$

The spectral theorem connects the $K(\omega)$ and the correlation function,

$$\langle B(t')A(t) \rangle = \langle A \rangle \langle B \rangle + \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{K(\omega) e^{-i\omega(t-t')}}{e^{\frac{\omega}{\Theta}} - \eta} d\omega. \quad (4)$$

Using the well-known expansion of the Heisenberg operator

$$e^{iHt} A e^{-iHt} = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \underbrace{[H, [H, \dots [H, A] \dots]]}_{n\text{-times}} \quad (5)$$

and comparing the time derivative at the moment $t = t' = 0$ in (3) and (5), we obtain the moments S_n of the spectral density function,

$$S_n = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \omega^n K(\omega) = (-1)^n \langle \underbrace{[[H, [H, \dots [H, A] \dots]]}_{n\text{-times}}, B \rangle_{\eta}. \quad (6)$$

The moments are a time-independent correlation function of a combination of the operators. It is possible to calculate it because the commutator relation of the Hamiltonian and the given operator is known.

The retarded Green function is described as follows:

$$\langle \langle A(t) | B(t') \rangle \rangle = -i\Theta(t) \langle [A(t), B(t')]_{\eta} \rangle. \quad (7)$$

Its Fourier transform, $G(E)$, obtained from a relation like (2), is related to the spectral density function,

$$G(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{K(\omega)}{E - \omega + i\varepsilon} d\omega \quad \text{where } \varepsilon \rightarrow 0^+. \quad (8)$$

If E is treated as a complex variable, then the $G(E)$ function will be analytical in the upper half-plane. Then,

$$G(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{K(\omega)}{E - \omega} d\omega \quad \text{for } \text{Im } E > 0. \quad (9)$$

The dispersion relation of the Green function permits us to find the spectral density, namely,

$$K(\omega) = -2 \text{Im } G(\omega + i\varepsilon). \quad (10)$$

2. Now the method of calculation will be presented. We will omit the proof, referring the reader to Akhiezer's monograph [2].

If the moments S_n of the given spectral density form a positive sequence, then the Green function of the relevant operators is a limit of the sequence

$$G(E) = \lim_{n \rightarrow \infty} G_n(E, \tau). \quad (11)$$

$G_n(E, \tau)$ is described by the fraction

$$G_n(E, \tau) = S_0 \frac{Q_{n+1}(E) - \tau Q_n(E)}{P_{n+1}(E) - \tau P_n(E)}. \quad (12)$$

The polynomials $P_n(E)$ are given by the determinant

$$P_0(E) = 1$$

$$P_n(E) = \frac{\sqrt{S_0}}{\sqrt{D_{n-1}D_n}} \begin{vmatrix} S_0 & S_1 & \dots & S_n \\ S_1 & S_2 & & S_{n+1} \\ \vdots & \vdots & & \vdots \\ S_{n-1} & S_n & & S_{2n-1} \\ 1 & E & & E^n \end{vmatrix} \quad \text{for } n \geq 1 \quad (13)$$

where $D_{-1} = D_0 = S_0$, and

$$D_n = \begin{vmatrix} S_0 & S_1 & \dots & S_n \\ S_1 & S_2 & \dots & S_{n+1} \\ \vdots & \vdots & & \vdots \\ S_n & S_{n+1} & \dots & S_{2n} \end{vmatrix} \quad \text{for } n \geq 1.$$

$P_n(E)$ is of order n with respect to E . The polynomial $Q_n(E)$, which is of order $n-1$ with respect to E , can be found from the relation

$$Q_n(E) = \frac{1}{2\pi S_0} \int_{-\infty}^{\infty} \frac{P_n(E) - P_n(\omega)}{E - \omega} K(\omega) d\omega \quad (14)$$

but in practice this will not be needed. The polynomials of the lowest order have the form

$$P_0(E) = 1; \quad P_1(E) = \frac{E - a_0}{b_0}$$

$$Q_0(E) = 0; \quad Q_1(E) = \frac{1}{b_0} \quad (15)$$

where

$$a_0 = \frac{S_1}{S_0}, \quad b_0 = S_2 - \frac{S_1^2}{S_0}.$$

The parameter τ admits all real values ($-\infty < \tau < \infty$). For a fixed E ($\text{Im } E > 0$), when τ runs from $-\infty$ to ∞ , the values of $G_n(E, \tau)$ form a circle in the upper half-plane

of G_n ($\text{Im } G_n(E, \tau) > 0$). The circle formed by function $G_n(E, \tau)$ lies entirely within the circle produced by $G_{n-1}(E, \tau)$ for the same E . The two circles have one point of osculation. This follows from the property

$$G_n(E, \infty) = G_{n-1}(E, 0). \quad (16)$$

If the problem is definite, then the circle formed by $G_n(E, \tau)$ (when τ admits the real axis) tends to a point in the limit $n \rightarrow \infty$. Thus the limit $G(E)$ does not depend on the parameter τ . The approximation procedure for the Green function consists in replacing $G(E)$ by $G_n(E, \tau)$ with a low value of n . In principle, a suitable choice of τ gives a better approximation of the Green function.

The fraction (12) can be expanded into the vulgar fractions (2)

$$G_n(E, \tau) = S_0 \frac{Q_{n+1}(E) - \tau Q_n(E)}{P_{n+1}(E) - \tau P_n(E)} = S_0 \sum_{i=1}^{n+1} \frac{\mu_i(\tau)}{E - E_i(\tau)}. \quad (17)$$

The numbers $E_i(\tau)$ ($i = 1, 2, \dots, n+1$) are roots of the following equation

$$P_{n+1}(E) - \tau P_n(E) = 0. \quad (18)$$

It can be proved that all roots of (18) are real and simple. The coefficients $\mu_i(\tau)$ can be obtained from a comparison of the two fractions in (17) or from the formula

$$\mu_i(\tau) = \frac{1}{\sum_{j=0}^n |P_j(E_i(\tau))|^2}. \quad (19)$$

We notice that the coefficients $\mu_i(\tau)$ are determined only by the first n polynomials $P_n(E_i(\tau))$. The roots $E_i(\tau)$ and coefficients $\mu_i(\tau)$ are related with the moments S_m :

$$S_m = S_0 \sum_{i=1}^{n+1} \mu_i(\tau) E_i(\tau)^m \text{ for } m = 0, 1, \dots, 2n$$

when $\tau \neq 0$

$$\text{or for } m = 0, 1, \dots, 2n+1 \quad (20)$$

when $\tau = 0$.

In particular, for $m = 0$

$$\sum_{i=1}^{n+1} \mu_i = 1. \quad (21)$$

The approximate calculation of the Green function can be carried out in the following way: Let the moments S_m ($m = 0, 1, \dots, 2n+2$) (6) be known. The polynomials $P_m(E)$ ($m = 0, 1, \dots, n+1$) may be formed from S_m . Then we find the roots $E_i(\tau)$ of equation (18) and the coefficients $\mu_i(\tau)$ (19). Using the relation (17) the approximate Green function can be obtained.

Example

Let the moments S_0, S_1, S_2 be given ($n = 0$). Using (17), we find the roots of (18),

$$E_1(\tau) = \frac{S_1}{S_0} + b_0\tau. \quad (22)$$

The value $\mu_1 = 1$ results from (19). In this approximation the Green function is

$$G_0(\tau) = \frac{S_0}{E - E_1(\tau)} \quad (23)$$

and the corresponding spectral density function

$$K(\omega) = 2\pi S_0 \delta(\omega - E_1). \quad (24)$$

Thus, undamped excitations are obtained.

If $2n + 2$ moments are given, then the equation (18) possesses $n + 1$ different roots $E_i(\tau)$. Each root is a real number. Thus, the spectral density function is made up of $(n + 1)$ δ -functions of different amplitudes,

$$K(\omega) = 2\pi S_0 \sum_{i=1}^{n+1} \mu_i \delta(\omega - E_i). \quad (25)$$

However, the appearance of $(n + 1)$ δ -functions does not mean that the true spectral density has $n + 1$ maxima. Moreover, the single δ -function, which approximates the density spectrum, does not have to be located at the maximum of $K(\omega)$. The arbitrary choice of parameter τ permits a shifting of the δ -function within some ω -interval. This interval decreases together with an increase of approximation order n . The number of δ -functions increases together with n and finally, at the limit $n = \infty$, forms the true density spectrum.

Usually, the spectral density is approximated by a Lorentzian function. Its maximum determines the energy of elementary excitations and its width represents the life-time of the excitations. In the present scheme we cannot obtain the lifetime of the excitations immediately because all roots of equation (18) are real.

3. The described procedure is still incomplete. We have yet to determine the parameter τ . One method assumes that $\tau = 0$. Another assumes such a value of τ for which the free energy, calculated in the given approximation, achieves minimum value. We shall discuss each of these ways.

The $\tau = 0$ method

For $\tau = 0$ the approximate Green function may be expressed by the continuous fraction

$$G_n(E, 0) = S_0 \frac{Q_{n+1}(E)}{P_{n+1}(E)} = \frac{S_0}{E - a_0 - \frac{b_0^2}{E - a_1 - \frac{b_1^2}{E - a_2 - \dots - \frac{b_{n-1}^2}{E - a_n}}} \quad (26)$$

where a_0 and b_0 are determined from (15), and the remaining coefficients can be found from the form of $Q_{n+1}(E)$ and $P_{n+1}(E)$. In particular, the continuous fraction of the zeroth and first order are

$$\frac{Q_1(E)}{P_1(E)} = \frac{1}{E - a_0}. \quad (27)$$

$$\frac{Q_2(E)}{P_2(E)} = \frac{1}{E - a_0 - \frac{b_0^2}{E - a_1}}. \quad (28)$$

When we know the moments (6), which are a combination of operators, it is easy to find the Green function. Moreover, some of the moments can be determined by the Green function to be found by the spectral theorem (2). However, very often the higher order moments cannot be obtained in this way. Then, a Green function of more complicated operator combination and an approach in the appropriate lower order must be applied.

In the paper [3] the decoupling of the density-density Green function for the many-body system was proposed. This decoupling process is equivalent to the zeroth order approximation by continuous fraction¹. Using the spectral theorem, the first moment S_1 from $G_0(E, 0)$ was calculated. In result, a self-consistent system of equations was obtained.

The "pseudoharmonic approximation" for a crystal lattice (4) is an example of similar type as above, but the moment S_1 cannot be determined from $G_0(E, 0)$ without additional approximations.

Tahir-Kehli and Jarrett [5] found the Green function $G_1(E, 0)$ of the Ising model for spin 1/2, in first order approximation. The spectral density from $G_1(E, 0)$ fulfilled four sum rules (S_0, S_1, S_2, S_3) in agreement with relations (20). However, this problem cannot be solved by the present scheme. $G_0(E, 0)$ is determined by two moments, S_0 and S_1 , but the spectral theorem gives only S_0 . Thus, the S_1 moments cannot be described self-consistently. The moment S_2 and S_3 have similar properties.

Kalashnikov and Fradkin [6] used this method for the superconductivity model (BCS) in zeroth order approximation.

The $\tau \neq 0$ method

It is well known that the free energy F of any system can be described by the two-particle Green function or corresponding correlation function. The τ -dependence of the approximate Green function involves the τ -dependence of the approximate free energy. Hence, we must find the approximate free energy $F(\tau)$ and minimize it with respect to τ .

¹ The even moments of position-position or density-density commutator correlation function vanish. Hence, the moments will be defined as

$$S_m = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega^2 \omega^{2m} K(\omega^2)$$

Assume that the Hamiltonian H can be divided into two parts, $H = H_0 + H_1$. H_0 is a part for which we are able to calculate the free energy. H_1 is a perturbation. Introduce the Hamiltonian $H(\lambda) = H_0 + \lambda H_1$, where λ is called the coupling constant ($H = H(1)$, $H_0 = H(0)$). Define the free energy as a function of the coupling constant

$$F(\lambda) = -\Theta \ln \text{Sp} \left(e^{-\frac{H(\lambda)}{\Theta}} \right) \quad (29)$$

and differentiate it with respect to λ :

$$\frac{\partial F(\lambda)}{\partial \lambda} = \frac{1}{Z(\lambda)} \text{Sp} \left\{ e^{-\frac{H(\lambda)}{\Theta}} \frac{dH(\lambda)}{d\lambda} \right\} \quad (30)$$

where

$$Z(\lambda) = \text{Sp} \left\{ e^{-\frac{H(\lambda)}{\Theta}} \right\}.$$

Integrating over λ from 0 to 1 we get

$$F = F(0) + \int_0^1 d\lambda \frac{1}{Z(\lambda)} \text{Sp} \left\{ e^{-\frac{H(\lambda)}{\Theta}} \frac{dH(\lambda)}{d\lambda} \right\}. \quad (31)$$

The average value $\left\langle \frac{dH(\lambda)}{d\lambda} \right\rangle_\lambda$ is easy to calculate. We must average $\frac{dH(\lambda)}{d\lambda}$ with the modified Hamiltonian $H(\lambda)$ instead of the true one, H . Of course, the average $\left\langle \frac{dH(\lambda)}{d\lambda} \right\rangle_\lambda$ may be calculated only approximately and, therefore it depends on τ . The value of τ can be found from the condition $\frac{dF(\tau)}{d\tau} = 0$.

In conclusion the author expresses his gratitude to Professor J. A. Janik for many discussions and helpful suggestions.

REFERENCES

- [1] D. N. Zubarev, *Uspekhi Fiz. Nauk* (USRR), **71**, 71 (1960).
- [2] N. I. Akhiezer, *Klassicheskaya problema momentov*, Gosud. izd. fiz.-mat. lit., Moskva 1961.
- [3] K. Parliński, *Physica* **51**, 299 (1971).
- [4] N. M. Plakida, T. Siklos, *Phys. Status Solidi*, **33**, 103 (1969).
- [5] R. A. Tahir-Kehli, H. S. Jarrett, *Phys. Rev.*, **180**, 544 (1969).
- [6] O. K. Kalashnikov, E. S. Fradkin, *Zhur. Eksp. Teor. Fiz.*, **55**, 607 (1968).