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LETTER TO THE EDITOR

Remarks on the Brillouin-Wigner perturbation theory

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Abstract. Some remarks on the Brillouin-Wigner degenerate perturbation theory are given together with an argument for the t - J model. It is shown that the two different types of the t - J model, which are frequently adopted in the current literature, in fact arise from the use of different Hilbert spaces.

A so-called t - J model, which is derived from the Hubbard model in the strong coupling limit, has recently been widely used to investigate the properties of high-temperature superconductors. However, the mathematical forms of the t - J model which many people adopt seem to be confused, i.e. some people use the expression [1]

$$H = -t \sum_{(ij)\sigma} (1 - n_{i-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} (1 - n_{j-\sigma}) + J \sum_{(ij)} (S_i \cdot S_j - \frac{1}{4} n_i n_j) \quad (1)$$

and others use another form [2]

$$H = -t \sum_{(ij)\sigma} c_{i\sigma}^\dagger c_{j\sigma} + J \sum_{(ij)} (S_i \cdot S_j - \frac{1}{4} n_i n_j). \quad (2)$$

Which of these is realistic? In this letter, we will address this issue in discussions of the Brillouin-Wigner (BW) perturbation theory [3]. Generally, one can obtain the t - J model from the Hubbard model in the limit of $U \gg t$ by using either the canonical transformation method [1] or the BW degenerate perturbation theory [2]. Whichever method is adopted, the form of the t - J model should be reasonably unique. Why do two different types (1) and (2) appear? In fact, as we will see below, (1) and (2) are written in different Hilbert spaces. On the other hand, the BW perturbation theory is still a powerful technique with which to treat a class of problems concerned with spin-orbital coupling under the actions of the crystal field in transition metals or alloys. Therefore, it is necessary to discuss the BW perturbation theory in detail.

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Consider a Hamiltonian of a system

$$H = H_0 + H_1 \quad (3)$$

where H_1 is very small with respect to H_0 , and can be regarded as a perturbation term. We further assume that H_0 is so sufficiently simple that its eigenvalue problem can be solved exactly

$$H_0 \phi_\alpha = E_\alpha^{(0)} \phi_\alpha \quad (4)$$

where the ground state of H_0 is degenerate. The ground-state energy of H_0 is denoted by $E^{(0)}$, and the corresponding eigenstates are labelled by ϕ_l, ϕ_j, \dots , etc. The excited eigenstates of H_0 , which may or may not be degenerate, are labelled by $\phi_\mu, \phi_\nu, \dots$, etc with corresponding eigenvalues $E_\mu^{(0)}, E_\nu^{(0)}, \dots$, etc. H satisfies the Schrödinger equation

$$(H_0 - E)\Psi = -H_1\Psi \quad (5)$$

with Ψ the eigenfunction and E the eigenvalue of H . As a result, Ψ can be written as a linear combination of ϕ_j and ϕ_μ , i.e.

$$\Psi = \Psi_{\text{ground}} + \Psi_{\text{excited}} = \sum_j a_j \phi_j + \sum_\mu a_\mu \phi_\mu. \quad (6)$$

Substituting equation (6) into (5), we find that

$$a_\nu = \frac{\langle \phi_\nu | H_1 | \Psi \rangle}{E - E_\nu^{(0)}}. \quad (7)$$

Equation (7) can also be rewritten as

$$a_\nu = \sum_j \left[\frac{\langle \phi_\nu | H_1 | \phi_j \rangle}{E - E_\nu^{(0)}} + \sum_\alpha \frac{\langle \phi_\nu | H_1 | \phi_\alpha \rangle \langle \phi_\alpha | H_1 | \phi_j \rangle}{(E - E_\nu^{(0)})(E - E_\alpha^{(0)})} + \dots \right] a_j. \quad (8)$$

Consequently, equation (6) becomes

$$\Psi = \sum_j a_j \left[\phi_j + \sum_\mu \phi_\mu \frac{\langle \phi_\mu | H_1 | \phi_j \rangle}{E - E_\mu^{(0)}} + \sum_{\mu, \nu} \phi_\mu \frac{\langle \phi_\mu | H_1 | \phi_\nu \rangle \langle \phi_\nu | H_1 | \phi_j \rangle}{(E - E_\mu^{(0)})(E - E_\nu^{(0)})} + \dots \right]. \quad (9)$$

Inserting equations (6) and (9) into equation (5), we obtain

$$\sum_j [\langle \phi_l | H_{\text{eff}} | \phi_j \rangle - E \delta_{lj}] a_j = 0 \quad (10)$$

where

$$\begin{aligned} \langle \phi_l | H_{\text{eff}} | \phi_j \rangle &= E^{(0)} \delta_{lj} + \langle \phi_l | H_1 | \phi_j \rangle + \sum_\mu \frac{\langle \phi_l | H_1 | \phi_\mu \rangle \langle \phi_\mu | H_1 | \phi_j \rangle}{E - E_\mu^{(0)}} \\ &+ \sum_{\mu, \nu} \frac{\langle \phi_l | H_1 | \phi_\mu \rangle \langle \phi_\mu | H_1 | \phi_\nu \rangle \langle \phi_\nu | H_1 | \phi_j \rangle}{(E - E_\mu^{(0)})(E - E_\nu^{(0)})} + \dots \end{aligned} \quad (11)$$

One can see that equation (10) is the same as the Schrödinger equation for the Hamiltonian H_{eff} which is often called the effective Hamiltonian of the system. Evidently, equation (10) is equivalent to

$$H_{\text{eff}}\Psi_{\text{ground}} = E\Psi_{\text{ground}}. \quad (12)$$

At this stage, we still have not made any approximations in the derivation, i.e. equations (11) and (12) are exact. Although we have reached a simple equation (12) for H_{eff} , we still cannot obtain the exact eigenvalue E because the exact form of H_{eff} cannot be written down easily. Generally speaking, one usually takes the following approximations [3] in equation (11): (i) $E - E_{\mu}^{(0)} \approx E^{(0)} - E_{\nu}^{(0)}$; and (ii) $\langle \phi_{\nu} | H_1 | \phi_j \rangle \ll (E^{(0)} - E_{\nu}^{(0)})$. By applying the two conditions, equation (12) can also be solved approximately. However, such an approximation is inappropriate, as discussed below. For the Hubbard model [4], if we take the correlation term as H_0 and the hopping term as H_1 , then from equation (11) one finds that the effective Hamiltonian (t - J model) is just equation (2), as shown in [2].

On the other hand, we can still obtain a similar equation to equation (12) in another way. Now we divide the full Hilbert space V into two subspaces V_0 and V_1 , i.e. $V = V_0 \oplus V_1$, where V_0 are spanned by the eigenvectors $\Psi_{\text{ground}} \equiv \Psi_0$, and V_1 are spanned by the eigenvectors $\Psi_{\text{excited}} \equiv \Psi_1$. We can also introduce two projection operators P and Q into the Hilbert space in the following way [5]

$$P : V \longrightarrow V_0 \quad Q : V \longrightarrow V_1 \quad (13)$$

or, equivalently,

$$P|\Psi\rangle = |\Psi_0\rangle = P|\Psi_0\rangle \quad Q|\Psi\rangle = |\Psi_1\rangle = Q|\Psi_1\rangle. \quad (14)$$

P and Q have the properties

$$P + Q = 1 \quad [P(Q), H_0] = 0. \quad (15)$$

At present, we use P and Q to perform on the two side of equation (5), and have

$$(E - H_0)|\Psi_0\rangle = PH_1P|\Psi_0\rangle + PH_1Q|\Psi_1\rangle \quad (16)$$

$$(E - H_0)|\Psi_1\rangle = QH_1P|\Psi_0\rangle + QH_1Q|\Psi_1\rangle. \quad (17)$$

By applying equation (17) to iterate equation (16), one obtains

$$H'_{\text{eff}}\Psi_0 = E\Psi_0 \quad (18)$$

with

$$H'_{\text{eff}} = E^{(0)} + PH_1P + \frac{PH_1QQH_1P}{E - H_0} + \dots \quad (19)$$

If one finds the operators P and Q satisfying equation (15), then H'_{eff} can be obtained. It may be seen that H'_{eff} varies slightly from H_{eff} . Obviously, equation (19) is written down in the full Hilbert space V , because the projection operators exist, whereas H_{eff} is written down in the Hilbert subspace V_0 . If we choose an appropriate form

[6] of P for the Hubbard model, then one finds that equation (1) may be obtained from equation (19) after ignoring some negligible terms. Thus we can state that the two somewhat distinct types (1) and (2) of the t - J model are, in fact, derived in different Hilbert spaces.

In addition, when one writes down an approximate form for the effective Hamiltonian up to a higher order than H_1^2 by using $E^{(0)}$ to replace E directly in equation (11), some terms are inappropriately missed. Assuming that $E - E^{(0)} = \varepsilon$ (ε is a small quantity), then $H_1 \sim \varepsilon$ [5]. Thus the third term on the right-hand side of equation (11) is proportional to

$$\sum_{\mu} \frac{\varepsilon^2}{E^{(0)} - E_{\mu}^{(0)}} - \sum_{\mu} \frac{\varepsilon^3}{(E^{(0)} - E_{\mu}^{(0)})^2}. \quad (20)$$

Usually, when we write down H_{eff} up to the order of H_1^2 , orders higher than $O(\varepsilon^3)$ are often neglected. It is easily observed that if one uses $E^{(0)}$ to replace E directly in equation (11), the second term of (20) is naturally dropped. This is correct up to the order of $O(H_1^2)$. However, if we include orders higher than $O(H_1^2)$ in equation (11), for instance if we go to the order of H_1^3 , then we find that it is no longer valid to use $E^{(0)}$ to replace E directly in equation (11). However, if such an approximation (which is usually adopted conventionally) is made, the second term of (20) will be missed whereas such a term has the same order as the main term of the order of H_1^3 , which should not be ignored. This can be seen from the fourth term on the right-hand side of equation (11) which is proportional to

$$\begin{aligned} & \sum_{\mu, \nu} \frac{\varepsilon^3}{(E^{(0)} - E_{\mu}^{(0)})(E^{(0)} - E_{\nu}^{(0)})} - \sum_{\mu, \nu} \frac{\varepsilon^4}{(E^{(0)} - E_{\mu}^{(0)})^2(E^{(0)} - E_{\nu}^{(0)})} \\ & - \sum_{\mu, \nu} \frac{\varepsilon^4}{(E^{(0)} - E_{\mu}^{(0)})(E^{(0)} - E_{\nu}^{(0)})^2}. \end{aligned} \quad (21)$$

Therefore, the correct form of H_{eff} up to the order of H_1^3 should be

$$\begin{aligned} \langle \phi_i | H_{\text{eff}} | \phi_j \rangle &= E^{(0)} \delta_{ij} + \langle \phi_i | H_1 | \phi_j \rangle + \sum_{\mu} \frac{\langle \phi_i | H_1 | \phi_{\mu} \rangle \langle \phi_{\mu} | H_1 | \phi_j \rangle}{E^{(0)} - E_{\mu}^{(0)}} \\ & - \sum_{\mu} \frac{\langle \phi_i | H_1^2 | \phi_{\mu} \rangle \langle \phi_{\mu} | H_1 | \phi_j \rangle}{(E^{(0)} - E_{\mu}^{(0)})^2} \\ & + \sum_{\mu, \nu} \frac{\langle \phi_i | H_1 | \phi_{\mu} \rangle \langle \phi_{\mu} | H_1 | \phi_{\nu} \rangle \langle \phi_{\nu} | H_1 | \phi_j \rangle}{(E^{(0)} - E_{\mu}^{(0)})(E^{(0)} - E_{\nu}^{(0)})} + O(H_1^4). \end{aligned} \quad (22)$$

A similar situation occurs for orders higher than $O(H_1^4)$, and those terms missed originally should be added to the expression for H_{eff} . Of course, all the above arguments are also suitable for equation (19).

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