Criterion for Validity of Many-Body Perturbation Theory of the Electron Gas

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The purpose of this paper is to point out the steps in conventional many-body perturbation theory which require separate, additional justification over and above convergence of the perturbation series. The questionable step is the cancellation of the renormalized energy shift by the chemical potential, neglecting any possible modification of the wave functions as well as state-dependent energy shifts.

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I have explored [1] the reasons for and the consequences of the fact that many-body perturbation theory as normally used in metals is not correct in a number of situations (which include at least all 2D Fermi systems). These papers have not been found, to my knowledge, to contain any errors. A number of other papers [2–4] have approached the problem of perturbation theory from a different point of view, attempting to find a difficulty with the convergence of the conventional series and have found no hint of the problems I have demonstrated. Some of these authors [2,3] and much of the community, feel that these papers are relevant to my work, although they are not, since my criticism applies to the method by which they proceed, not to whether that procedure converges on its own terms. It seems that it would be useful to return to the *basis* of perturbation theory and show which steps can go wrong.

One of the confusing points in this imbroglio is that many people are under the misapprehension that the known exact solution [5] of the one-dimensional system can be essentially obtained by resumming perturbation theory. This is not the case; some aspects are roughly correct, others—such as the sharp Mott-Hubbard gap at general n, the selection rules coupling charge and spin excitations, and certain coupling constant identities [6]—are not. Thus the implication that difficulties necessarily show up as a failure of convergence is questionable.

For definiteness we study the Hubbard model

$$\mathcal{H}=\sum_{ij\sigma}^{N} t_{ij}c_{i\sigma}^{*}c_{j\sigma}+U\sum_{i\sigma}n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i\sigma}n_{i\sigma}\,, \tag{1}$$

but any model with short-range interactions is subject to similar problems. It is important to retain the finite system and go to the infinite N limit only at the end.

$$\mathcal{H}_0=\sum_{ij}t_{ij}c_{i\sigma}^{*}c_{j\sigma}-\mu N$$

is diagonalized with boundary conditions by a set of Bloch waves k, and μ is adjusted so that the interaction does not change the density.

$$\mathcal{H}_0=\sum_{k\sigma}(\epsilon_k-\mu')c_{k\sigma}^{*}c_{k\sigma}\quad(\mu'\simeq\mu+\delta\mu)\,. \tag{2}$$

Hypothetically, the space of occupied states, determined by the set of k's, does not change as a result of interactions. Now one expands in a diagram series in U with perturbation denominators involving the ϵ_k.

It is already here that the crucial step takes place. The simplest diagrams are those of Hartree type which represent pure, elastic forward scattering of two particles $k\sigma$ and $k'\sigma'$ (there are no Fock diagrams for the model [1]). All ground state diagrams can be thought of as renormalizations of this basic diagram and as leading to a renormalized ground state energy $\propto\langle n_{k\sigma}\rangle\langle n_{k'\sigma'}\rangle$.

But for reasons we will shortly explore, the Hartree terms are hard to deal with so the following trick is usually employed. The subset of self-energy diagrams is taken which are irreducible with respect to on-shell, forward scattering (i.e., $k\sigma,k'\sigma'\rightarrow k\sigma,k'\sigma'$). We call their sum $\delta\mu$. This shift in the mean energy is to be compensated by a shift in chemical potential, which "of course" must be the same for all k's at the Fermi surface.

Then we use as our new perturbing potential $U\sum_i n_{i\uparrow}n_{i\downarrow}-\delta\mu\sum_{k\sigma}n_{k\sigma}$, and this perturbing potential apparently leads to no Hartree-type diagrams. The self-energy as a function of k,ω is calculated with this potential, and vanishes at the Fermi surface. μ is later retrieved by a coupling constant integration trick, so that it never, apparently, has to be calculated directly. All diagrams now involve only interactions with finite momentum and energy transfer.

Another way to express this process is that it is the way of solving the renormalized Hartree-Fock wave equations for the wave functions of the quasiparticles. The reason it is expected to be possible to do it this way is translational symmetry: The wave functions must be Bloch waves, and they must, apparently, be the *same* Bloch waves as the unperturbed ones obtained in Eq. (2). But, in fact, this is true only in the limit $N\rightarrow\infty$ and we must check that the $1/N$ corrections are not finite.

When put this way it seems manifestly obvious that the procedure needs justification. In particular, if one adds a spin-up particle in state $k\uparrow$, this has no effect on other spin-up particles, but gives a mean potential shift for $k'\downarrow$. Thus "$\delta\mu$" becomes spin dependent, and cannot be identical for all states at the Fermi surface. The wave equation for spin-down particles differs from that for spin-up ones. That this kind of effect of change in the wave equation

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occurs in finite systems is obvious, and it is essential to make sure that it does not persist as $N \to \infty$. It is clearly essential not to finesse the solution of this Hartree-Fock problem by artificially replacing the effects of on-shell scattering by a chemical potential shift.

One problem with the on-shell scattering problem is that when the phase shift is finite the effective potential is ambiguous, as pointed out many years ago by Fukuda and Newton [7], and the boundary conditions must be taken into account in order to determine the correct wave functions and energy shift. This is the problem which my papers have dealt with.

I will not reiterate the calculations here but quote results and principles. As pointed out above, the bare vertex U leads to disaster, since the s-wave phase shift is finite and an $\uparrow$ spin electron is equivalent to an ordinary scattering potential for all down-spin electrons, which in turn leads to the well-known "infrared catastrophe," and $Z \to 0$ for the added electron [8] by an argument given in my previous Letter [9].

In doing this calculation one realizes that the boundary conditions play a role. The scatterer is somewhere interior to the system, so that in most of space, and in particular in the asymptotic region near the boundaries, there is no scattering potential. The scatterer causes a local perturbation which provides a new boundary condition on the wave equation at the origin in relative coordinates. This boundary condition shifts the actual k' values of the $\downarrow$ spin particles so that the two spaces of momentum values are not quite the same (if the boundary conditions are real; if outgoing, particles move in and out through the boundaries; the effect is the same) [10]. These shifts in k' also lead to energy shifts (the phase shift, as observed in Ref. [7]) which contribute to the self-energy of particle $k\uparrow$ and which are not contained in perturbation theory, since they are primarily kinetic energy terms, and depend on boundary conditions which are absent from perturbation theory. These terms come from the self-consistent determination of the wave functions, which had been bypassed in the conventional methodology as explained above.

In many cases the situation is saved by allowing the scattering electron to respond dynamically, i.e., to recoil. If this recoil leads to "effective range theory" with a finite scattering length a, none of the wave functions need undergo a finite momentum shift relative to the granularity $1/L$ in momentum space. This is the case assumed without proof by Abrikosov, Gorkov, and Dzialoshinkii [11] and it is proved in the limit $N/V \to 0$ by Yang and co-workers and by Galitskii [12]. (Later, Bloom [13] proved an equivalent result for the $N/V \to 0$ limit in 2D.) It turns out that at least one criterion of validity is that the phase shift δ vanish as the relative momentum $Q = k - k' \to 0$.

My proof for 2D shows that the $N/V \to 0$ limit is unique and that in general, in 2D, there is a finite shift in the wave vectors of all electrons relative to their spacing when one electron is added. The origin of this result lies in the demonstration of a finite on-shell T matrix, which has been confirmed in fact in Ref. [3]. This reference differs from my result only in the physical discussion of this Letter; there is no controversy about the finite phase shift. I have shown how this involves a radical modification of the elementary excitation spectrum; the solution of the difficulty involves new physics which has been discussed elsewhere.

The question of 3D is still open. In one article I have given a general argument that the strong coupling Hubbard model is not a Fermi liquid, from a somewhat intuitive guess that a projective transformation of the Hilbert space cannot be carried out perturbatively in U. This conjecture finds some support in the physical properties of a number of substances, which are suggestively bizarre or mysterious. The evidence that moderate interactions or free particle bands lead, in 3D, to convergent perturbation theory and Fermi liquid behavior is strong but cannot be conclusive; the question must be investigated in detail.

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