Renormalized vs. unrenormalized perturbation-theoretical approaches to the Mott transition

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Abstract

I employ an exactly soluble toy model to investigate why unrenormalized perturbation theory works better than fully self-consistent approaches in describing the correlation-driven metal-insulator transition.

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Theoretical works on the Mott transition [1] have mainly focused on the Hubbard model of strongly correlated electrons [2]. Its main feature is the competition between itineracy and an on-site repulsion $U$. At half filling and zero temperature, the Hubbard model exhibits a metal-insulator transition at some critical value $U_c$. At the moment, the only unified framework for describing the various features and phases associated with this Mott transition is provided by the dynamical mean-field theory [3], which becomes exact in the limit of infinite dimensions introduced by Metzner and Vollhardt [4]. However, the dynamical mean-field equations cannot be solved exactly, and various approximate numerical schemes have been employed to study their intricate structure. An important approximation for describing the half-filled Hubbard model and the Mott transition is the so-called iterated perturbation theory (IPT). This approximation succeeds to simultaneously capture the quasiparticle resonance and the incoherent lower and upper Hubbard bands. Partly based on the IPT, Zhang, Rozenberg, and Kotliar put forward a scenario for the Mott transition, in which the width of the quasiparticle resonance vanishes linearly in $U - U_c$ while its height remains unchanged, as the transition point $U_c$ is approached from below [5]. This scenario was directly confirmed by the projective self-consistent technique of Moeller et al. [6]. Yet, the IPT is based on second-order perturbation theory in $U$ and might therefore be suspected to be inferior to perturbation-theoretical schemes that are either fully self-consistent or involve larger classes of diagrams. Self-consistent perturbation expansions have the advantage of conserving exact symmetries and their respective conservation laws [7]. Therefore, some authors have adopted a self-consistent approach from the outset [8,9]. Others, by contrast, have pointed out early on that fully self-consistent approaches seem to work worse than ordinary perturbation theory [10]. They relied on weak-coupling studies of the half-filled single-impurity Anderson model [11–13]. Meanwhile, there is a large body of numerical evidence, that, at least not too close to the Mott transition, IPT is quantitatively accurate [3,14]. But it is not fully understood why leading-order perturbation theory works so well, whereas seemingly more elaborate self-consistent approaches notoriously fail to properly describe the insulating phase and their precursor effects.
It is the purpose of this paper, to shed some light on this issue by considering an exactly solvable toy model that crudely captures some features of the Mott transition. This model is defined by the following Hamiltonian:

\[ \hat{H} = U (\hat{n}_\uparrow - \frac{1}{2}) (\hat{n}_\downarrow - \frac{1}{2}) + V \sum_\sigma (f_\sigma^+ c_\sigma + c_\sigma^+ f_\sigma), \]  

where \( \hat{n}_\sigma \equiv c_\sigma^+ c_\sigma \). It describes a correlated \( c \) orbital hybridizing with an \( f \) orbital at zero energy. At half filling and zero temperature, particle-hole symmetry guarantees that the Green’s function depends on three independent parameters only,

\[ G(z) = \frac{1}{2} \left( \frac{a_j}{z - \epsilon_j} + \frac{a_j}{z + \epsilon_j} \right), \]  

\[ \epsilon_1 = \frac{1}{4} \left( \sqrt{U^2 + 64V^2} - \sqrt{U^2 + 16V^2} \right), \]  

\[ \epsilon_2 = \frac{1}{4} \left( \sqrt{U^2 + 64V^2} + \sqrt{U^2 + 16V^2} \right), \]  

\[ a_1 = \frac{1}{4} \left( 1 - \frac{U^2 - 32V^2}{\sqrt{(U^2 + 64V^2)(U^2 + 16V^2)}} \right), \]

where \( z \) is a complex frequency and \( a_2 = 1/2 - a_1 \). At \( V = 0 \), the Green’s function has two poles of equal weight at \( \pm U/2 \) and thus represents an insulator. For \( V \ll U \), \( \epsilon_1 \simeq 6V^2/U \), \( \epsilon_2 \simeq U/2 + 10V^2/U \), and \( a_1 \simeq 18V^2/U^2 \). The appearance of spectral weight at \( \pm \epsilon_1 \), close to the “Fermi level” at zero energy, is the best approximation to a metallic phase which is possible within our model. In the limit \( V \to 0 \), this spectral weight disappears, thus simulating a “metal-to-insulator transition.” If we think of the two \( \delta \) function contributions at \( \pm \epsilon_1 \) to the single-particle spectrum as representing the quasiparticle resonance (QPR), its total weight is given by \( Z \equiv 2a_1 \simeq 36V^2/U^2 \) and its width by \( T^* \equiv 2\epsilon_1 \simeq ZU/3 \).

From Eqs. (2)-(5), we obtain the noninteracting Green’s function \( G_0 \) and the self-energy \( \Sigma(z) \equiv G_0^{-1}(z) - G^{-1}(z) \),

\[ G_0(z) = \frac{1}{2} \left( \frac{1}{z - V} + \frac{1}{z + V} \right) = \frac{z}{z^2 - V^2}, \]

\[ \Sigma(z) = \frac{U^2}{8} \left( \frac{1}{z - 3V} + \frac{1}{z + 3V} \right) = \frac{U^2}{4} \frac{z}{z^2 - 9V^2}. \]

The first quantity is completely determined by \( V^2 \), while the second one also depends on \( U^2 \). The poles of the self-energy at \( \pm 3V \) are precursors of the \( 1/z \) pole of the insulating
phase. Note, that close to the transition point, \( V \ll U \), these poles are located in the gap of the single-particle spectrum between the QPR and the “Hubbard bands”. The reason is that, while the width \( T^* \) of the QPR collapses linearly in \( ZU \), the self-energy poles move more slowly towards the Fermi level at \( \omega = 0 \), according to a \( \sqrt{ZU} \) behavior. Note, that at least the dependences on \( Z \) are in agreement with the scenario of Ref. [5] on the Mott transition in the Hubbard model: There, \( T^* \sim ZD \), while the self-energy acquires poles at about \( \pm \sqrt{Z} D \) (\( D \) is the half bandwidth of the bare band).

We now consider the self-energy as a functional of the noninteracting Green’s function. Eqs. (6) and (7) imply

\[
i\Sigma(t) = U^2[iG_0(t)]^3,
\]

which means that the IPT approximation [3] becomes exact in our toy model.

Next, we ask what we would obtain in leading-order self-consistent perturbation theory. The leading-order skeleton diagram for the self-energy is equivalent to Eq. (8), except that we have to replace the noninteracting Green’s function by the fully renormalized one of Eq. (2). In the frequency domain, we obtain

\[
\Sigma(z) = U^2 \left[ a_1^3 \left( \frac{1}{z - 3\epsilon_1} + \frac{1}{z + 3\epsilon_1} \right) + 3a_1^2a_2 \left( \frac{1}{z - (2\epsilon_1 + \epsilon_2)} + \frac{1}{z + (2\epsilon_1 + \epsilon_2)} \right) + 3a_1a_2^2 \left( \frac{1}{z - (\epsilon_1 + 2\epsilon_2)} + \frac{1}{z + (\epsilon_1 + 2\epsilon_2)} \right) + a_2^3 \left( \frac{1}{z - 3\epsilon_2} + \frac{1}{z + 3\epsilon_2} \right) \right].
\]

As we approach the “insulating phase,” \( V \to 0 \), only poles at \( \pm 3U/2 \) with residues \( U^2/8 \) survive. This approximation, therefore, fails to bring about the \( 1/z \) pole characteristic of the insulating phase. Its failure to account for the insulating phase becomes even more evident if we translate the result of Eq. (9) into a single-particle spectral function. For \( V = 0 \), we find a spurious \( \delta \) function contribution at the Fermi level, that carries 90% of the spectral weight. This problem is not specific to our toy model. In the context of the infinite-dimensional
Hubbard model, second-order self-consistent perturbation theory suffered from exactly the same flaws [8]. There, too, it always predicts the existence of a QPR with a spectral weight that tends to be too large.

Finally, we express the exact self-energy as a functional of the full Green’s function (4) with the goal of elucidating why its expansion in powers of $U$ might break down as we approach the “transition point,” $V \to 0$. The skeleton expansion of the self-energy is obtained by regarding $G$ as a functional of $G_0$ and $U$, $G[G_0,U]$, and by substituting the inverted functional $G_0[G,U]$ into $\Sigma[G_0,U]$. This requires the knowledge of $G$ for an arbitrary $G_0$ and thus the solution of the most general impurity model, which is hopeless. Nevertheless, the essential element of the skeleton expansion is that the self-energy is viewed as a functional of $G$ and $U$ rather than $G_0$ and $U$. Since in our case, $G_0$ is parametrized by a single parameter, $V^2$, straightforward perturbation theory consists in expanding $\Sigma(V^2, U)$ in powers of $U$. By contrast, renormalized perturbation theory corresponds to first trading $V^2$, which completely determines $G_0$, for one of the three parameters that determine the Green’s function (2), say, $\epsilon_1$, and afterwards expanding $\Sigma(\epsilon_1, U)$ in powers of $U$. The procedure of going over from $\Sigma(V^2, U)$ to $\Sigma(\epsilon_1, U)$ corresponds to performing a Legendre transformation. Each of the Eqs. (3)-(5) can be solved uniquely for $V^2$:

\begin{align}
V^2 &= \frac{\epsilon_1}{18} \left( 10\epsilon_1 + \sqrt{64\epsilon_1^2 + 9U^2} \right), \quad (10) \\
V^2 &= \frac{\epsilon_2}{18} \left( 10\epsilon_2 - \sqrt{64\epsilon_2^2 + 9U^2} \right), \quad (11) \\
V^2 &= \frac{9 - 40a_1 + 80a_1^2 + 3(4a_1 - 1)\sqrt{9 - 8a_1 + 16a_1^2}}{1024a_1(1 - 2a_1)} U^2. \quad (12)
\end{align}

Depending on which of these equations we insert into Eq. (7), we obtain a different parametrization of $\Sigma[G,U]$. If renormalized perturbation theory were well-behaved all the way down to the transition point, $V \to 0$, all parametrizations of $\Sigma[G,U]$ would also be well-behaved when expanded in powers of $U$. Yet, the expansion of $\Sigma(\epsilon_1, U)$ in powers of $U$ involves an expansion of the square root in Eq. (10) in powers of $U/\epsilon_1$, which converges only for $U < 8\epsilon_1/3$. But since $\epsilon_1 \to 0$ as $V \to 0$, this expansion has zero radius of con-
vergence as one approaches the point $V = 0$, which is the analog of the Mott transition. More specifically, this expansion fails to converge for $V^2/U^2 \leq (5 + 4\sqrt{2})/64 \simeq 0.167$, or for $Z \leq 9(4 - \sqrt{2})/28 \simeq 83\%$. This result indicates that the skeleton expansion of the self-energy is increasingly misbehaved as the Mott transition is approached, even though the actual range of convergence seems to be widely underestimated by our toy model.

In summary, I have demonstrated within a simple toy model that neither second-order self-consistent perturbation theory nor a skeleton expansion of the self-energy to all orders in $U$ can account for the Mott transition properly. While the former approach always predicts a metallic phase and overestimates the spectral weight of the quasiparticle resonance, the latter one fails to converge in the vicinity of the transition. By contrast, ordinary leading-order perturbation theory in $U$ is well-behaved and, in our simple toy model, even turns out to be exact.

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