Analytic properties of insulating solution of half-filled Hubbard model

A.V. Joura, D. O. Demchenko, J. K. Freericks
Physics Department, Georgetown University
Washington, DC, 20057

Financial support
National Science Foundation DMR-0210717
Office of Naval Research, N00014-99-1-0328

Motivation

- "the precise mechanism for the disappearance of the insulating solution at U_{c1}, the behavior of the gap at this point, and the value of U_{c1} have not yet been fully settled" (Georges et al., RMP 68, 1996)
- Only numerical solutions are obtained so far
- We need better understanding whether the hypercubic lattice has some advantages over the Bethe lattice or not

Hubbard model for D=∝

$$G(i\omega_n) = \int_{-\infty}^{+\infty} \frac{\rho(\varepsilon)d\varepsilon}{i\omega_n - \widetilde{\Sigma}(i\omega_n) - \varepsilon} \quad , \quad \rho(\varepsilon) = e^{-\varepsilon^2} / \sqrt{\pi}$$

$$\widetilde{\Sigma}(i\omega_n) = \widetilde{G}_0^{-1}(i\omega_n) - G^{-1}(i\omega_n)$$

$$G(\tau) = -< Tc(\tau)c^+(0) >_{Seff[\widetilde{G}_0]}$$

where shifted quantities $\widetilde{G}_0^{-1} \equiv G_0^{-1} - \frac{U}{2}$ and $\widetilde{\Sigma} = \Sigma - \frac{U}{2}$

and we call $A_0(\varepsilon) = -\mathrm{Im}(\widetilde{G}_0(\varepsilon))/\pi$ a spectral function

We have THREE UNKNOWN functions: $\widetilde{G}_0(\omega)$, $\widetilde{\Sigma}(\omega)$ and $G(\omega)$

Iterative Perturbation Theory

- We are going to work on real axis after doing analytic continuation $i\omega_n \to \omega + i\delta$
- We'll replace last equation by expression for self-energy in second order perturbation theory (IPT approximation): $\widetilde{\Sigma} = -U^2 \widetilde{G}_0^2(-\tau)\widetilde{G}_0(\tau)$

Analytic continuation to real frequencies gives (see Kajuter et al, PRB 53, 1996)

$$\widetilde{\Sigma}(\omega) = U^2 \int_0^{+\infty} d\varepsilon_1 d\varepsilon_2 d\varepsilon_3 \frac{A_0(\varepsilon_1)A_0(-\varepsilon_2)A_0(-\varepsilon_3)}{\omega - \varepsilon_1 - \varepsilon_2 - \varepsilon_3 + i\delta} + U^2 \int_0^{+\infty} d\varepsilon_1 d\varepsilon_2 d\varepsilon_3 \frac{A_0(\varepsilon_1)A_0(-\varepsilon_2)A_0(-\varepsilon_3)}{\omega + \varepsilon_1 + \varepsilon_2 + \varepsilon_3 + i\delta}$$

Iterative Perturbation Theory (continued)

- $\widetilde{G}_0(\omega)$ and $\widetilde{\Sigma}(\omega)$ have a pole at zero frequency
- Most general form of free-particle Green's function in the insulating phase:

$$\widetilde{G}_0(\omega) = \frac{\alpha}{\omega + i\delta} + \widetilde{G}_{0,reg}(\omega)$$

with corresponding spectral function

$$A_0(\omega) = \alpha\delta(\omega) + \Delta(\omega)$$

where $\Delta(\omega) = -\mathrm{Im}(\widetilde{G}_{0,reg}(\omega))/\pi$ is a symmetric function

Region of small frequencies ($\omega << 1$)

- Our 2 integral equations become local in ω :

$$\tilde{\Sigma}(\omega + i\delta) = \frac{U^2}{4} \cdot \frac{\alpha^3}{\omega + i\delta} + \frac{3U^2\alpha^2}{4}\tilde{G}_{0,reg} + O(\omega)$$

$$\mathrm{Re}(G^{-1} + \tilde{\Sigma}) = \left(1 + \frac{2}{U^2\alpha^3}\right)\omega + O(\omega^3)$$

$$\mathrm{Im}(G^{-1} + \tilde{\Sigma}) = \mathrm{Im}(\tilde{\Sigma})\left(-\frac{8\omega^2}{U^4\alpha^6} + O(\omega^4)\right) + \pi\rho\left(-\frac{\alpha^3 U^2}{4\omega} + O(\omega)\right)\left(\frac{\alpha^6 U^4}{16\omega^2} + O(1)\right)$$

- Last equation remains unchanged:

$$\tilde{G}_0(\omega)\left(G^{-1}(\omega) + \tilde{\Sigma}(\omega)\right) - 1 = 0$$

Solution in power series w.r.t. $\omega << 1$

$$\tilde{\Sigma}_1(\omega) = \frac{\alpha^3 U^2}{4\omega} + O(\omega)$$

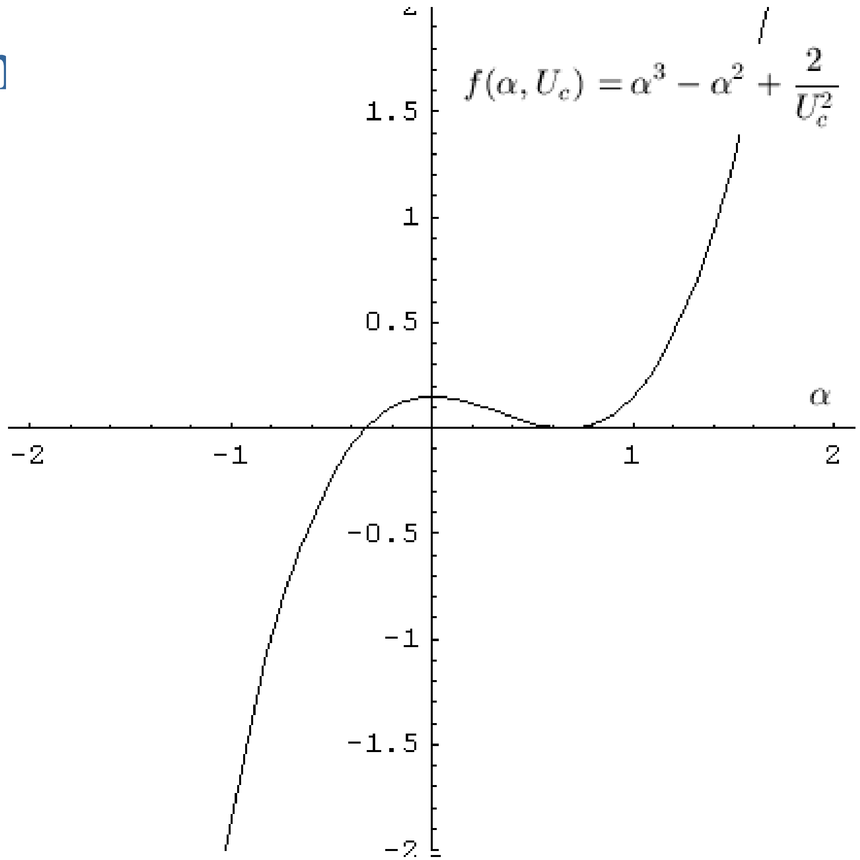
$$\tilde{\Sigma}_2(\omega) = \left(-\frac{3\alpha^4}{8\sqrt{\pi}(1-\alpha)^3(3\alpha-2)\omega^4} + O\left(\frac{1}{\omega^2}\right)\right) e^{-\frac{\alpha^2}{4(1-\alpha)^2\omega^2}+O(1)} - \frac{\pi\alpha}{2(1-\alpha)}\delta(\omega)$$

where α for a given U is determined by the equation:

$$\left(1 + \frac{2}{U^2\alpha^3}\right)\alpha = 1$$

- This equation for α coincides with one, found before for the Bethe lattice (see Rozenberg et al., PRB 49, 1994), if we consider Bethe lattice of same bandwidth
- Solution with $\alpha > 0$ exists only for $U > U_{c1} = 3\sqrt{3/2}$

Existence of insulating solution



α for a given U is determined by the equation:

$$f(\alpha) = \alpha^3 - \alpha^2 + \frac{2}{U^2} = 0$$

- Solution with $\alpha > 0$ exists only for $U > U_{c1} = 3\sqrt{3/2} \approx 3.67$
- U_{c1} is in good agreement with the numerical value $U_{c1} \approx 3.7$ (see Georges et al., PRB 48, 1993)
- The Bethe and the hypercubic lattice of same bandwidth have same $U_{c1} \approx 5.2$ for same bandwidth ($D_{hc}=D_{Bethe}/2=1$)

Conclusions

- We found analytic solutions to the half-filled Hubbard model in DMFT within IPT approximation close Fermi energy (Green's function, self energy)
- We found analytic expression for critical value of the field U_{c1} when insulating solution disappears
- It's shown that when insulating solution disappears a pole in self energy disappears discontinuously
- We found that critical value U_{c1} is same for the hypercubic and the Bethe lattice of same bandwidth
- We found analytic expression for effective relaxation time close to the pole in self energy

Thank you for your attention

- I would also like to thank Dr. Barbara Jones and IBM Almaden Research Center for hosting me while this work was being performed.