Assignments 8, 9 e 11

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1 Assigment 8

1.1 Problem 1

Temos que $\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij}$, $\{\hat{a}_i, \hat{a}_j^\dagger \hat{a}_j\} = \delta_{ij} a_j$ e $\{\hat{a}_i^\dagger, \hat{a}_j^\dagger \hat{a}_j\} = -\delta_{ij}\hat{a}_j^\dagger$. Além disso, das relações $[\hat{a}, \hat{b}\hat{c}] = \{\hat{a}, \hat{b}\}\hat{c} - \hat{b}\{\hat{a}, \hat{c}\}$ ou $[\hat{a}\hat{b}, \hat{c}] = \hat{a}\{\hat{b}, \hat{c}\} - \{\hat{a}, \hat{c}\}\hat{b}$, temos que

$$[\hat{a}_1, \hat{a}_1^\dagger \hat{a}_2] = \{\hat{a}_1, \hat{a}_1^\dagger\}\hat{a}_2 - \hat{a}_1^\dagger\{\hat{a}_1, \hat{a}_2\} = \hat{a}_2 - 0 = \hat{a}_2.$$

1.1.1

Com a hamiltoniana $\hat{H} = \sum_{k=1}^{2} \epsilon_k \hat{a}_k^\dagger \hat{a}_k - \lambda(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1)$, segue então que $[\hat{a}_1, \hat{H}] = \epsilon_1 \hat{a}_1 - \lambda \hat{a}_2$. Analogamente para $[\hat{a}_2, \hat{H}]$, obtemos da equação de Heisenberg:

$$i\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\hat{a}_1 \\ \hat{a}_2\end{pmatrix} = \begin{pmatrix}\epsilon_1 & -\lambda \\ -\lambda & \epsilon_2\end{pmatrix}\begin{pmatrix}\hat{a}_1 \\ \hat{a}_2\end{pmatrix} = M\begin{pmatrix}\hat{a}_1 \\ \hat{a}_2\end{pmatrix}. \tag{1}$$

Por M ser simétrica, sabemos que pode ser diagonalizada ortonormalmente. Assim, escrevemos $M = U \operatorname{diag}(\omega_1, \omega_2)\, U^T$, onde parametrizamos

$$U = \begin{pmatrix}\cos\theta & \sin\theta \\ -\sin\theta & \cos\theta\end{pmatrix}.$$

1.1.2

A solução da equação 1.1.1 é dada por $\mathbf{\hat{a}}(t) = U \operatorname{diag}(e^{-i\omega_1 t}, e^{-i\omega_2 t})\, U^T\, \mathbf{\hat{a}}(0)$. Portanto

$$\begin{pmatrix}\hat{a}_1(t) \\ \hat{a}_2(t)\end{pmatrix} = \begin{pmatrix}\cos\theta & \sin\theta \\ -\sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}e^{-i\omega_1 t}\cos\theta & -e^{-i\omega_1 t}\sin\theta \\ e^{-i\omega_2 t}\sin\theta & e^{-i\omega_2 t}\cos\theta\end{pmatrix}\begin{pmatrix}\hat{a}_1(0) \\ \hat{a}_2(0)\end{pmatrix} =$$

$$\begin{pmatrix}e^{-i\omega_1 t}\cos^2\theta + e^{-i\omega_2 t}\sin^2\theta & (e^{-i\omega_2 t} - e^{-i\omega_1 t})\sin\theta\cos\theta \\ (e^{-i\omega_2 t} - e^{-i\omega_1 t})\sin\theta\cos\theta & e^{-i\omega_2 t}\cos^2\theta + e^{-i\omega_1 t}\sin^2\theta\end{pmatrix}\begin{pmatrix}\hat{a}_1(0) \\ \hat{a}_2(0)\end{pmatrix}.$$

1.1.3

No limite em que $\lambda = 0$, a matriz M já é diagonal. Nesse caso, temos que $U = \mathbb{1}$ e $\theta = 0$. Nesse caso, a solução se reduz a $\hat{a}_k(t) = e^{-i\epsilon_k t}\hat{a}_k(0)$, que é a solução da *free-hamiltonian*, onde só existe uma oscilação de fase trivial.

1.1.4

Com a solução obtida em 1.1.2, podemos calcular $\hat{n}_k(t) = \hat{a}_k^\dagger(t)\hat{a}_k(t)$. Para o caso do $\hat{n}_1$ temos

$$\hat{n}_1(t) = \Big\{\big[e^{i\omega_1 t}\cos^2\theta + e^{i\omega_2 t}\sin^2\theta\big]\hat{a}_1^\dagger(0) + \big[(e^{i\omega_2 t} - e^{i\omega_1 t})\sin\theta\cos\theta\big]\hat{a}_2^\dagger(0)\Big\}$$

$$\times\big\{\big[e^{-i\omega_1 t}\cos^2\theta + e^{-i\omega_2 t}\sin^2\theta\big]\hat{a}_1(0) + \big[(e^{-i\omega_2 t} - e^{-i\omega_1 t})\sin\theta\cos\theta\big]\hat{a}_2(0)\big\}.$$

Fazendo essa bagunça:

$$\begin{aligned}\boxed{\hat{n}_1(t)} = &\big\{\cos^4\theta + 2\cos^2\theta\sin^2\theta\,\cos[(\omega_2-\omega_1)t] + \sin^4\theta\big\}\,\hat{a}_1^\dagger(0)\hat{a}_1(0) + \\ &\big\{2\sin^2\theta\cos^2\theta\,(1-\cos[(\omega_2-\omega_1)t])\big\}\,\hat{a}_2^\dagger(0)\hat{a}_2(0) + \\ &\big\{\sin\theta\cos\theta\big[\big(1+e^{i(\omega_2-\omega_1)t}\big)\sin^2\theta - \big(1-e^{-i(\omega_2-\omega_1)t}\big)\cos^2\theta\big]\big\}\,\hat{a}_1^\dagger(0)\hat{a}_2(0) + \\ &\big\{\sin\theta\cos\theta\big[\big(1+e^{-i(\omega_2-\omega_1)t}\big)\sin^2\theta - \big(1-e^{i(\omega_2-\omega_1)t}\big)\cos^2\theta\big]\big\}\,\hat{a}_2^\dagger(0)\hat{a}_1(0).\end{aligned}$$

A expressão para $\hat{n}_2(t)$ é obtida trocando $1 \leftrightarrow 2$.

1.2 Problem 2

1.2.1

Chamando $\lambda = V_d - V_x$, temos

$$[\hat{a}_1, \hat{H}] = \epsilon\hat{a}_1 + \lambda(\hat{a}_1\hat{a}_1^\dagger\hat{a}_2^\dagger\hat{a}_2\hat{a}_1 - \hat{a}_1^\dagger\hat{a}_1\hat{a}_2^\dagger\hat{a}_2\cancelto{0}{\hat{a}_1}) = (\epsilon_1 + \lambda\hat{a}_2^\dagger\hat{a}_2)\,\hat{a}_1.$$

Analogamente, $[\hat{a}_2, \hat{H}] = (\epsilon_2 + \lambda\hat{a}_1^\dagger\hat{a}_1)\,\hat{a}_2$.

1.2.2

As equações de movimento são

$$\begin{cases} i\frac{\mathrm{d}\hat{a}_1}{\mathrm{d}t} = (\epsilon_1 + \lambda\hat{n}_2)\,\hat{a}_1 \\ i\frac{\mathrm{d}\hat{a}_2}{\mathrm{d}t} = (\epsilon_2 + \lambda\hat{n}_1)\,\hat{a}_2, \end{cases} \tag{2}$$

onde $\hat{n}_k = \hat{a}_k^\dagger\hat{a}_k$.

1.2.3

Note que a equação de movimento para $\hat{a}_1^\dagger$ é

$$i\frac{\mathrm{d}\hat{a}_1^\dagger}{\mathrm{d}t} = -(\epsilon_1 + \lambda\hat{n}_2)\,\hat{a}_1^\dagger$$

Perceba então que

$$i\frac{\mathrm{d}\hat{n}_1}{\mathrm{d}t} = i\frac{\mathrm{d}\hat{a}_1^\dagger}{\mathrm{d}t}\,\hat{a}_1 + \hat{a}_1^\dagger\,i\frac{\mathrm{d}\hat{a}_1}{\mathrm{d}t} = -(\epsilon_1 + \lambda\hat{n}_2)\hat{a}_1^\dagger\hat{a}_1 + \hat{a}_1^\dagger(\epsilon_1 + \lambda\hat{n}_2)\hat{a}_1 = 0.$$

O mesmo vale para $\hat{n}_2$. Portanto, $\hat{n}_k(t) = \hat{a}_k^\dagger(0)\hat{a}_k(0)$ é um operador constante.

Com essa observação, *à princípio*, é possível resolver as equações de movimento para $\hat{a}_1(t)$ e $\hat{a}_2(t)$ analiticamente. A solução é dada pela exponencial de um operador constante:

$$\hat{a}_1(t) = e^{-i\left[\epsilon_1+\lambda\hat{a}_2^\dagger(0)\hat{a}_2(0)\right]}\hat{a}_1(0) \quad \text{e} \quad \hat{a}_2(t) = e^{-i\left[\epsilon_2+\lambda\hat{a}_1^\dagger(0)\hat{a}_1(0)\right]}\hat{a}_2(0).$$

Agora, $\langle\hat{n}_k\rangle(t) = \left\langle\hat{a}_k^\dagger(0)\hat{a}_k(0)\right\rangle = \text{cte}$.

1.2.4

Na aproximação de *mean-field*, separamos $\hat{H} = \hat{H}_0 + \hat{V}$, onde $\hat{H}_0 = \sum_{k=1}^{2}\epsilon_k\hat{a}_k^\dagger\hat{a}_k$ e $\hat{V} = \lambda\,\hat{n}_1\hat{n}_2$. Então expandimos $\hat{V}$, substituindo $\hat{n}_k = \langle\hat{n}_k\rangle + \hat{\delta}_k$ e ignoraremos termos de segunda ordem $O(\hat{\delta}_k\hat{\delta}_\ell)$.

O potencial de *mean-field* é

$$V_{\text{MF}} = \lambda\Big(\langle\hat{n}_1\rangle\,\hat{n}_2 + \langle\hat{n}_2\rangle\,\hat{n}_1 - \langle\hat{n}_1\rangle\langle\hat{n}_2\rangle\Big).$$

Agora podemos calcular os comutadores $[\hat{a}_k, \hat{H}]$ e obter novamente as equações de movimento. Porém, outra maneira mais direta é fazer diretamente na equação exata 2 a aproximação de *mean-field* $n_k\hat{a}_\ell = \langle n_k\rangle\,\hat{a}_\ell$.

A solução é muito parecida com o que já obtivemos:

$$\hat{a}_1(t) = e^{-i\left[\epsilon_1+\lambda\left\langle\hat{a}_2^\dagger(0)\hat{a}_2(0)\right\rangle\right]}\hat{a}_1(0) \quad \text{e} \quad \hat{a}_2(t) = e^{-i\left[\epsilon_2+\lambda\left\langle\hat{a}_1^\dagger(0)\hat{a}_1(0)\right\rangle\right]}\hat{a}_2(0).$$

2 Assignment 9

2.1 Problem 1

Ah, é muito fácil substituir G^R e G^A nas equações e verificar que

$$\left[\frac{\mathrm{d}}{\mathrm{d}t} - H\right]G(\mathbf{r}t,\mathbf{r}'t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t').$$

Agora, temos que G^R e G^A são independentes pois $G^R(\mathbf{r}t,\mathbf{r}'t') = 0$ para $t < t'$ enquanto que $G^A(\mathbf{r}t,\mathbf{r}'t') = 0$ para $t > t'$.

2.2 Problem 2

Temos que

$$\frac{1}{\omega + i\eta} = \frac{\omega}{\omega^2+\eta^2} - i\pi\,\frac{\eta/\pi}{\omega^2+\eta^2}.$$

Integrando sobre uma função teste f, temos que

$$\begin{aligned}\lim_{\eta\to 0}\int_{-\infty}^{\infty}\frac{f(\omega)\,\mathrm{d}\omega}{\omega+i\eta} &= \lim_{\eta\to 0}\int_{-\infty}^{\infty}\frac{f(\omega)\,\omega\,\mathrm{d}\omega}{\omega^2+\eta^2} \;-\; i\pi\,\lim_{\eta\to 0}\int_{-\infty}^{\infty}f(\omega)\,\frac{\eta/\pi}{\omega^2+\eta^2}\,\mathrm{d}\omega\\ &= P.V.\int_{-\infty}^{\infty}\frac{f(\omega)}{\omega}\,\mathrm{d}\omega - i\pi f(0).\end{aligned}$$

Isso mostra que

$$\lim_{\eta\to 0}\frac{1}{\omega+i\eta} = P.V.\left(\frac{1}{\omega}\right) - i\pi\delta(\omega).$$

3 Assignment 11

3.1 Problem 1

Assumindo que $\Sigma^{(0)}(\omega^+) = \Lambda - i\Delta$, com Λ e Δ constantes, temos que

$$\overline{G}^R_{d\sigma}(\omega^+) = \frac{\Big[\omega - \big(\epsilon_0 + \Lambda + U\left\langle \hat{n}_{d\overline{\sigma}} \right\rangle\big)\Big] - i\Big[\Delta + \eta\Big]}{\Big[\omega - \big(\epsilon_0 + \Lambda + U\left\langle \hat{n}_{d\overline{\sigma}} \right\rangle\big)\Big]^2 + \Big[\Delta + \eta\Big]^2}.$$

Portanto

$$\left\langle \hat{n}_{d\sigma} \right\rangle = \int_{-\infty}^{\epsilon_F} A_{d\sigma}(\omega)\,\mathrm{d}\omega = \frac{1}{\pi}\lim_{\eta\to 0}\int_{-\infty}^{\epsilon_F} \frac{(\Delta + \eta)\,\mathrm{d}\omega}{\Big[\omega - \big(\epsilon_0 + \Lambda + U\left\langle \hat{n}_{d\overline{\sigma}} \right\rangle\big)\Big]^2 + \Big[\Delta + \eta\Big]^2}$$

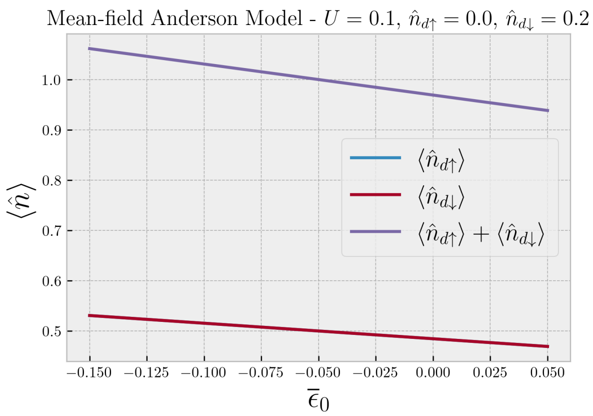
$$= \frac{1}{\pi}\int_{-\infty}^{\epsilon_F} \frac{1}{1 + \left[\frac{\omega - (\overline{\epsilon}_0 + U\left\langle \hat{n}_{d\overline{\sigma}} \right\rangle)}{\Delta}\right]^2}\frac{\mathrm{d}\omega}{\Delta}.$$

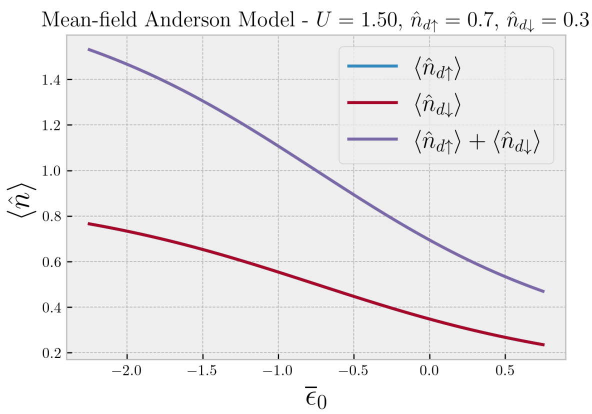
Substituindo $\xi = \frac{\omega - (\overline{\epsilon}_0 + U\left\langle \hat{n}_{d\overline{\sigma}} \right\rangle)}{\Delta}$ e aproximando a energia de Fermi $\epsilon_F \approx 0$, obtemos

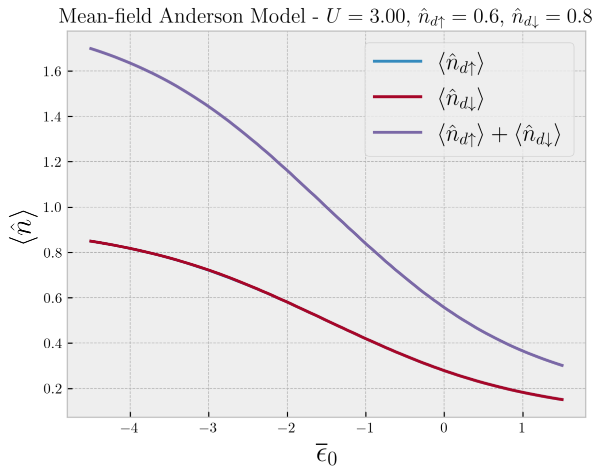
$$\left\langle \hat{n}_{d\sigma} \right\rangle = \frac{1}{\pi}\int_{-\infty}^{-\frac{\overline{\epsilon}_0 + U\left\langle \hat{n}_{d\overline{\sigma}} \right\rangle}{\Delta}} \frac{\mathrm{d}\xi}{1 + \xi^2} = \frac{1}{2} - \frac{1}{\pi}\arctan\left(\frac{\overline{\epsilon}_0 + U\left\langle \hat{n}_{d\overline{\sigma}} \right\rangle}{\Delta}\right).$$

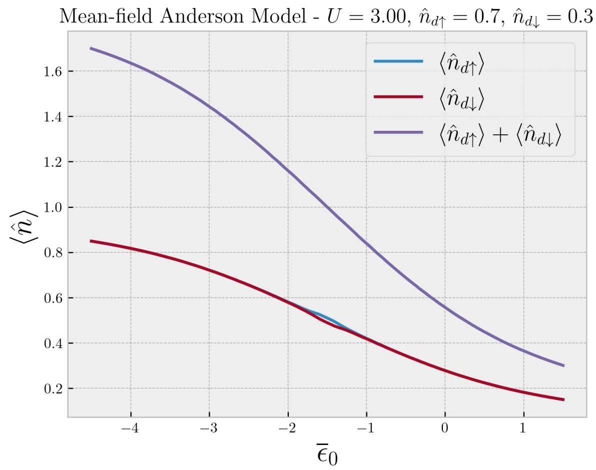
3.2 Problem 2

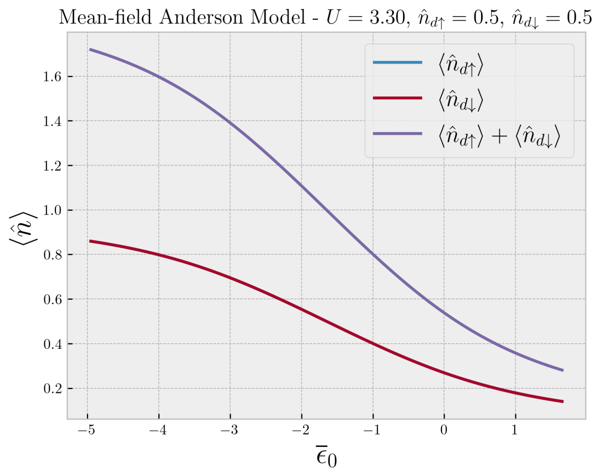
Não entendi o comentário de tomar a média da iteração anterior no código do modelo de Anderson. Tempo 43:22 no vídeo da Aula 11.

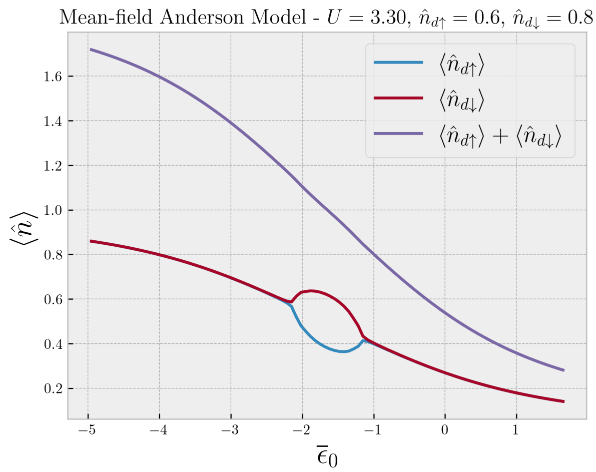


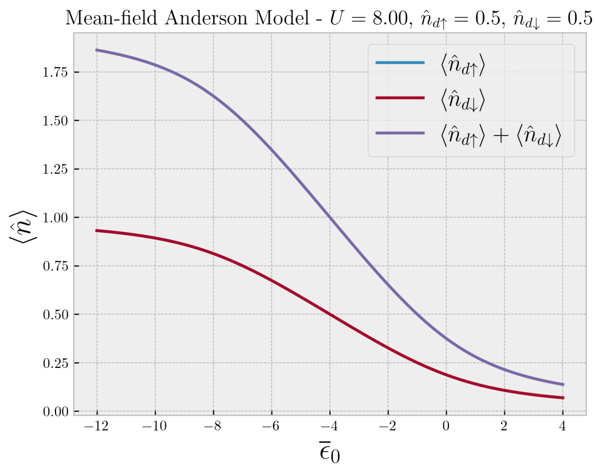


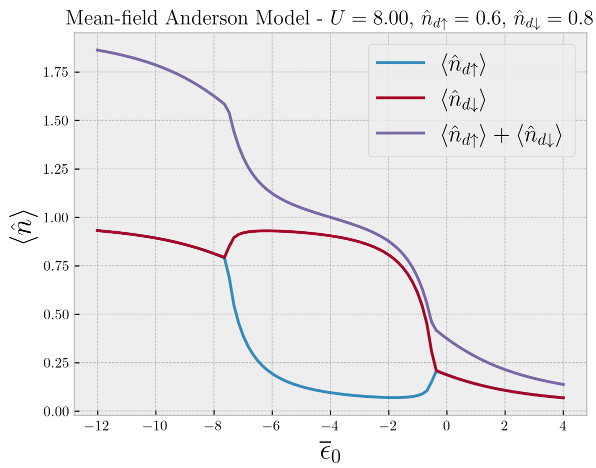

Mean-field Anderson Model - $U = 3.00$, $\hat{n}_{d\uparrow} = 0.6$, $\hat{n}_{d\downarrow} = 0.8$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\bar{\epsilon}_0$

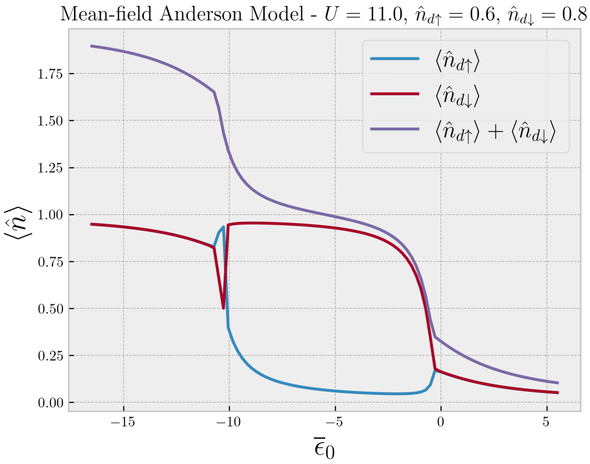

Mean-field Anderson Model - $U = 3.00$, $\hat{n}_{d\uparrow} = 0.7$, $\hat{n}_{d\downarrow} = 0.3$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\bar{\epsilon}_0$

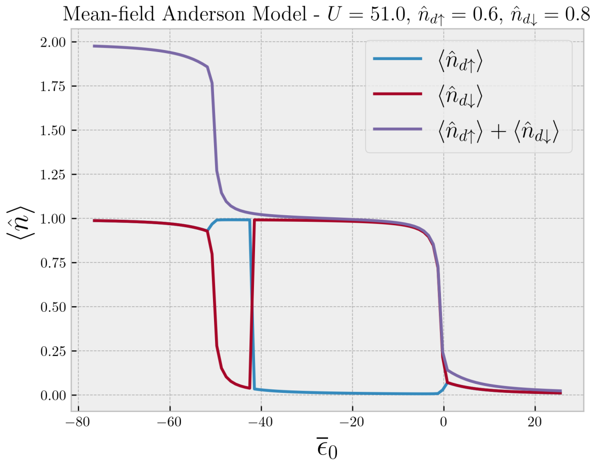

Mean-field Anderson Model - $U = 3.30$, $\hat{n}_{d\uparrow} = 0.5$, $\hat{n}_{d\downarrow} = 0.5$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\bar{\epsilon}_0$

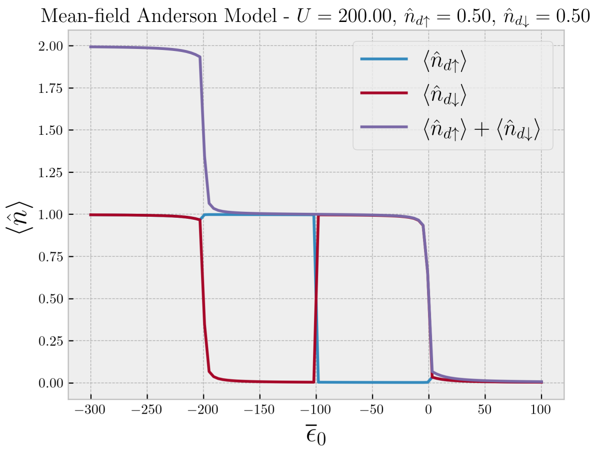

Mean-field Anderson Model - $U = 3.30$, $\hat{n}_{d\uparrow} = 0.6$, $\hat{n}_{d\downarrow} = 0.8$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\bar{\epsilon}_0$

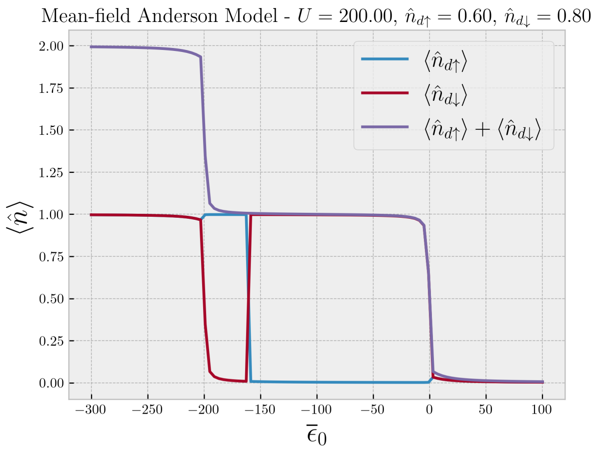

Mean-field Anderson Model - $U = 8.00$, $\hat{n}_{d\uparrow} = 0.5$, $\hat{n}_{d\downarrow} = 0.5$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\bar{\epsilon}_0$

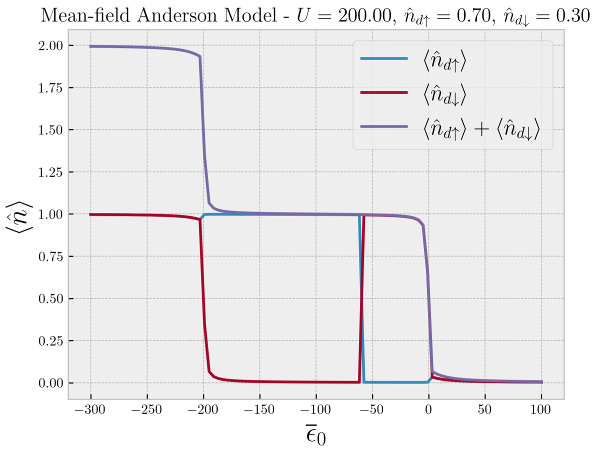

Mean-field Anderson Model - $U = 8.00$, $\hat{n}_{d\uparrow} = 0.6$, $\hat{n}_{d\downarrow} = 0.8$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\bar{\epsilon}_0$

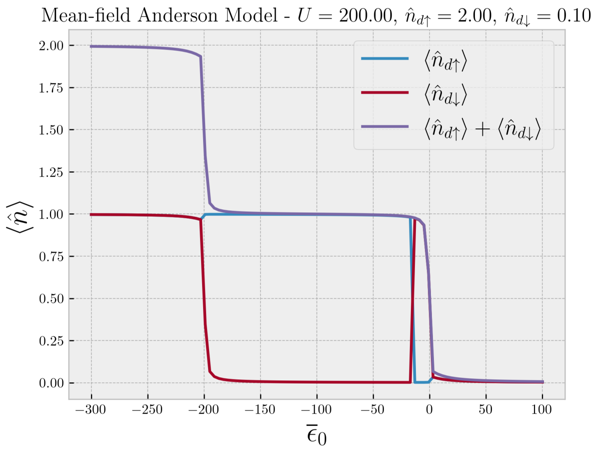

Mean-field Anderson Model - $U = 11.0$, $\hat{n}_{d\uparrow} = 0.6$, $\hat{n}_{d\downarrow} = 0.8$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\overline{\epsilon}_0$


Mean-field Anderson Model - $U = 51.0$, $\hat{n}_{d\uparrow} = 0.6$, $\hat{n}_{d\downarrow} = 0.8$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\overline{\epsilon}_0$


Mean-field Anderson Model - $U = 200.00$, $\hat{n}_{d\uparrow} = 0.50$, $\hat{n}_{d\downarrow} = 0.50$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\overline{\epsilon}_0$


Mean-field Anderson Model - $U = 200.00$, $\hat{n}_{d\uparrow} = 0.60$, $\hat{n}_{d\downarrow} = 0.80$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\overline{\epsilon}_0$


Mean-field Anderson Model - $U = 200.00$, $\hat{n}_{d\uparrow} = 0.70$, $\hat{n}_{d\downarrow} = 0.30$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\overline{\epsilon}_0$


Mean-field Anderson Model - $U = 200.00$, $\hat{n}_{d\uparrow} = 2.00$, $\hat{n}_{d\downarrow} = 0.10$
$\langle \hat{n}_{d\uparrow} \rangle$
$\langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n}_{d\uparrow} \rangle + \langle \hat{n}_{d\downarrow} \rangle$
$\langle \hat{n} \rangle$
$\overline{\epsilon}_0$