The Anderson Impurity Model as a Derivative of the Hubbard Model

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  Hubbard model with impurity

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Models: Anderson Impurity Model

Model of band electrons and one impurity with spin and charge degree

$$\overline{H} = \sum_{\overline{k},\sigma} \overline{k}\, n_{\overline{k},\sigma} + \sum_{\overline{k},\sigma} \left(\overline{V} c^{\dagger}_{\overline{k},\sigma} d_{\sigma} + \overline{V} d^{\dagger}_{\sigma} c_{\overline{k},\sigma} \right) + \epsilon_d \sum_{\sigma} n_{d,\sigma} + \overline{U} n_{d,\uparrow} n_{d,\downarrow}$$

Bethe ansatz equations by Wiegmann (1980)

$$\mathrm{e}^{\mathrm{i}\overline{k}_j l} \frac{\overline{k}_j - \epsilon_d - \frac{\mathrm{i}}{2}\overline{V}^2}{\overline{k}_j - \epsilon_d + \frac{\mathrm{i}}{2}\overline{V}^2} = \prod_{\alpha=1}^{M} \frac{g\left(\overline{k}_j\right) - \overline{\lambda}_{\alpha} + \frac{\mathrm{i}}{2}}{g\left(\overline{k}_j\right) - \overline{\lambda}_{\alpha} - \frac{\mathrm{i}}{2}}, \qquad \text{where } g\left(\overline{k}\right) = \frac{\left(\overline{k} - \epsilon_d - \overline{U}/2\right)^2}{\overline{U}\,\overline{V}^2}$$

$$\prod_{j=1}^{N} \frac{\overline{\lambda}_{\alpha} - g\left(\overline{k}_j\right) + \frac{\mathrm{i}}{2}}{\overline{\lambda}_{\alpha} - g\left(\overline{k}_j\right) - \frac{\mathrm{i}}{2}} = - \prod_{\beta=1}^{M} \frac{\overline{\lambda}_{\alpha} - \overline{\lambda}_{\beta} + \mathrm{i}}{\overline{\lambda}_{\alpha} - \overline{\lambda}_{\beta} - \mathrm{i}}, \qquad \text{energy } E = \sum_{j=1}^{N} \overline{k}_j$$

Derivation rather involved (coordinate Bethe ansatz, single particle waves are not plane waves...)

There are much simpler models: chains with “transparent impurities”

The Anderson impurity model (AIM) looks very different, but...

Models: Hubbard Model

Model of band electrons on lattice with on-site Coulomb repulsion

$$H_{\text{Hubbard}} = -\sum_{j=1}^{L}\Big(\sum_{\sigma=\uparrow,\downarrow}(c_{j+1,\sigma}^{\dagger}c_{j,\sigma}+c_{j,\sigma}^{\dagger}c_{j+1,\sigma})+Un_{j,\uparrow}n_{j,\downarrow}\Big)$$

Bethe ansatz equations (Lieb+Wu 1968)

$$e^{\mathrm{i}k_jL} = \prod_{l=1}^{M}\frac{\lambda_l-\sin k_j-\mathrm{i}\frac{U}{4}}{\lambda_l-\sin k_j+\mathrm{i}\frac{U}{4}},$$

$$\prod_{j=1}^{K}\frac{\lambda_l-\sin k_j-\mathrm{i}\frac{U}{4}}{\lambda_l-\sin k_j+\mathrm{i}\frac{U}{4}} = -\prod_{m=1}^{M}\frac{\lambda_l-\lambda_m-\mathrm{i}\frac{U}{2}}{\lambda_l-\lambda_m+\mathrm{i}\frac{U}{2}}.$$

Non difference type R-matrix (two XX 6VM + coupling, Shastry 1986)

$$\begin{aligned}\check{R}(\lambda,\mu) &= \cos(\lambda+\mu)\cosh(h(\lambda,U)-h(\mu,U))\,\check{r}(\lambda-\mu)\\ &\quad+\cos(\lambda-\mu)\sinh(h(\lambda,U)-h(\mu,U))\,\check{r}(\lambda+\mu)\,\sigma_{1,\uparrow}^{z}\sigma_{1,\downarrow}^{z},\end{aligned}$$

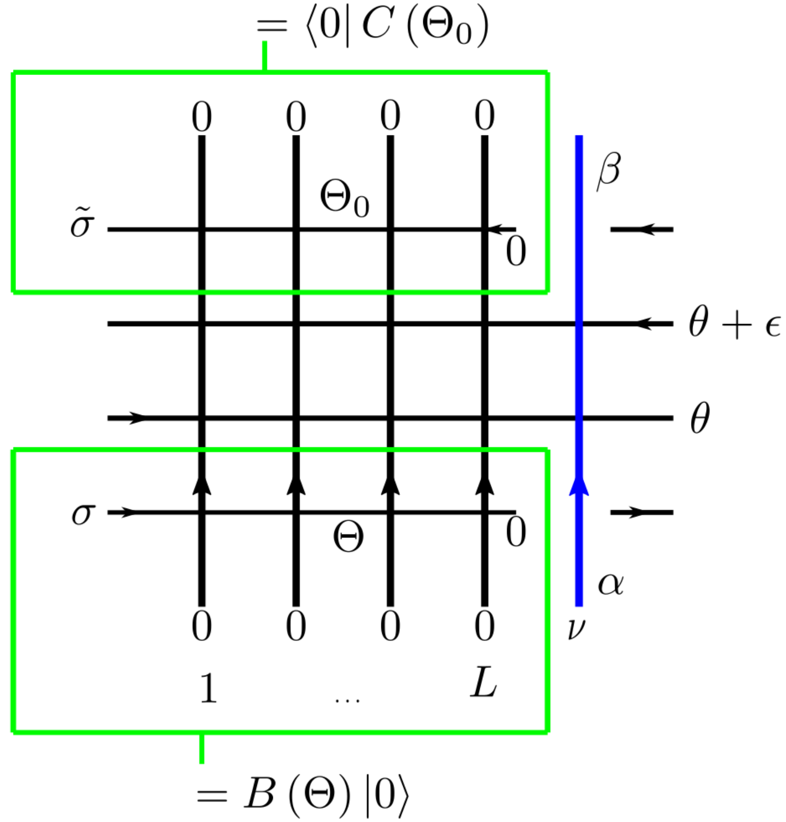
Matrix Elements $H \leftrightarrow TT$

Hamiltonian limit

$$T(\theta)\overline{T}(\theta+\epsilon) = \mathrm{e}^{-\epsilon H} + O(\mathrm{e}^{-c \cdot L}) \qquad (H \text{ local only for } \theta = 0)$$

Matrix elements of H from those of product of transfer matrices

$$\langle\Theta_0| \otimes \langle\beta|\, e^{-\epsilon H}\, |\Theta\rangle \otimes |\alpha\rangle =$$

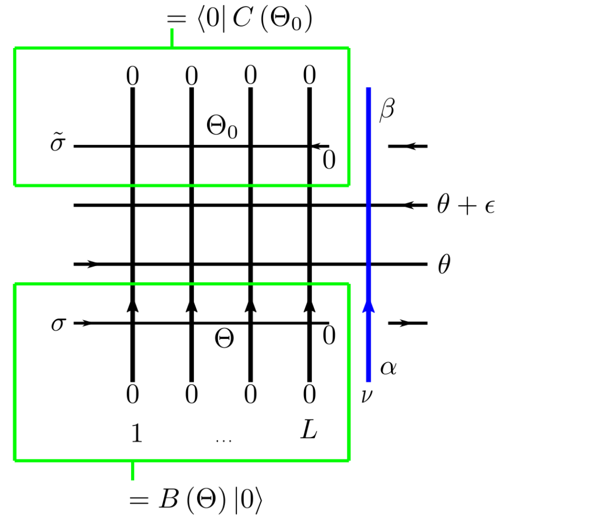


+periodic boundary conditions on horizontal lines

Matrix Elements of TT in Thermodynamic Limit

Matrix elements of $T(\theta)\overline{T}(\theta+\epsilon)$
in thermodynamic limit

$$\langle\Theta_0|\otimes\langle\beta|\, e^{-\epsilon H}\,|\Theta\rangle\otimes|\alpha\rangle =$$



+periodic boundary conditions on horizontal lines

- by use of column-to-column transfer matrices T_0 and T_i of size $2^2 4^2 \times 2^2 4^2$
- only 4 eigenvalues are maximal: 1, $\mathrm{e}^{\mathrm{i}k_{\rm in}}$, $\mathrm{e}^{-\mathrm{i}k_{\rm out}}$, $\mathrm{e}^{\mathrm{i}(k_{\rm in}-k_{\rm out})}$
- $\mathrm{Tr}(T_0^L T_i) = \sum_{n=1}^{4} \Lambda_n^L \langle n|T_i|n\rangle$, then derivative w.r.t. ϵ

Spectral parameters on 4 horizontal lines and 2 vertical lines

$$H_1 = \frac{\mathrm{i}\overline{V}\,\overline{U}^{1/2} a}{\sqrt{\mathrm{i}8\cos k_{\rm in}}},\ H_2 = 1+t,\ H_3 = 1+t_\epsilon,\ H_4 = \frac{\mathrm{i}\overline{V}\,\overline{U}^{1/2} a}{\sqrt{\mathrm{i}8\cos k_{\rm out}}},\ V_0 = 1,\ V_i = \frac{1}{2}\overline{V} a^{1/2}$$

Matrix Elements

Hybridization (conduction electron $\leftrightarrow$ impurity electron)

$$\begin{aligned} \langle\{k_{\text{out}},\uparrow\}|\; H \;|\{d,\uparrow\}\rangle &= [2+\mathrm{i}\cos(k_{\text{out}})]\cdot\overline{V}a^{1/2} \\ \langle\{d,\uparrow\}|\; H \;|\{k_{\text{in}},\uparrow\}\rangle &= [2-\mathrm{i}\cos(k_{\text{in}})]\cdot\overline{V}a^{1/2} \end{aligned}$$

(same for $\downarrow$)

Onsite matrix elements at impurity

$$\begin{aligned} \langle\{d,0\}|\; H \;|\{d,0\}\rangle &= 0 \\ \langle\{d,\uparrow\}|\; H \;|\{d,\uparrow\} &= -\overline{U}a \\ \langle\{d,\downarrow\}|\; H \;|\{d,\downarrow\} &= -\overline{U}a \\ \langle\{d,\uparrow\downarrow\}|\; H \;|\{d,\uparrow\downarrow\} &= 0 \end{aligned}$$

Conduction electrons energy: $e(k) = 2\cos k$

In continuum limit ($k_{\text{in}}, k_{\text{out}} \sim \pi/2$):
same matrix elements as for $\overline{H} - \mu_0 N$ with $\mu_0 = \epsilon_d + \overline{U}/2$.

BA Equations for Hubbard + Impurity / Continuum Limit I

The Bethe ansatz equations for the modified 1d Hubbard model are

$$\mathrm{e}^{\mathrm{i}k_j L} \mathrm{e}^{2h(v_i)} \frac{\frac{z_-(k_j)}{z_+(v_i)} + 1}{z_-(v_i) - z_-(k_j)} = \prod_{l=1}^{M} \frac{\lambda_l - \sin k_j - \mathrm{i}\frac{U}{4}}{\lambda_l - \sin k_j + \mathrm{i}\frac{U}{4}},$$

$$\prod_{j=1}^{K} \frac{\lambda_l - \sin k_j - \mathrm{i}\frac{U}{4}}{\lambda_l - \sin k_j + \mathrm{i}\frac{U}{4}} = -\prod_{m=1}^{M} \frac{\lambda_l - \lambda_m - \mathrm{i}\frac{U}{2}}{\lambda_l - \lambda_m + \mathrm{i}\frac{U}{2}}.$$

The additional phase factor in the first set – due to the impurity – evaluates to

$$\mathrm{i}\,\mathrm{e}^{2h(v_i)} \frac{\frac{z_-(k_j)}{z_+(v_i)} + 1}{z_-(v_i) - z_-(k_j)} = \frac{k_j - \pi/2 - \frac{a}{2}\left(\overline{U} + \mathrm{i}\overline{V}^2\right)}{k_j - \pi/2 - \frac{a}{2}\left(\overline{U} - \mathrm{i}\overline{V}^2\right)} = \frac{\overline{k}_j + \frac{1}{2}\left(\overline{U} + \mathrm{i}\overline{V}^2\right)}{\overline{k}_j + \frac{1}{2}\left(\overline{U} - \mathrm{i}\overline{V}^2\right)}$$

where for the last equality we used the continuum limit for momenta close to $\frac{\pi}{2}$

$$\overline{k}_j \equiv -\frac{k_j - \pi/2}{a}$$

BA Equations for Hubbard + Impurity / Continuum Limit II

In the continuum limit ($a \to 0$) we rename / use

$$\overline{\lambda}_\alpha \equiv -\frac{2}{U}(\lambda_\alpha - 1), \qquad \sin k_j = 1 - \frac{1}{2}\overline{k}_j^2 a^2$$

and find

$$e^{i\overline{k}_j l} \frac{\overline{k}_j + \frac{1}{2}\left(\overline{U} - i\overline{V}^2\right)}{\overline{k}_j + \frac{1}{2}\left(\overline{U} + i\overline{V}^2\right)} = \prod_{\alpha=1}^{M} \frac{g\left(\overline{k}_j\right) - \overline{\lambda}_\alpha + \frac{i}{2}}{g\left(\overline{k}_j\right) - \overline{\lambda}_\alpha - \frac{i}{2}},$$

$$\prod_{j=1}^{N} \frac{\overline{\lambda}_\alpha - g\left(\overline{k}_j\right) + \frac{i}{2}}{\overline{\lambda}_\alpha - g\left(\overline{k}_j\right) - \frac{i}{2}} = -\prod_{\beta=1}^{M} \frac{\overline{\lambda}_\alpha - \overline{\lambda}_\beta + i}{\overline{\lambda}_\alpha - \overline{\lambda}_\beta - i}, \qquad \text{where } g\left(\overline{k}\right) = \frac{\overline{k}^2}{\overline{U}\,\overline{V}^2}$$

The energy is obtained from

$$E = \frac{1}{a}\sum_{j=1}^{N} \cos k_j = \sum_{j=1}^{N} \overline{k}_j$$

Replacing $\overline{k}_j \to \overline{k}_j - \mu_0 = \overline{k}_j - \epsilon_d - \overline{U}/2$ gives Wiegmann's result

TBA for Hubbard

- Impurity does not change the TBA-equations of the Hubbard model, which follow from Takahashi's equations and the minimization of the Gibbs free energy

$$\ln \zeta(k) = -2\beta \cos k - 4\beta \int_{\mathbb{R}} \mathrm{d}y\, s(\sin k - y) \mathrm{Re} \sqrt{1 - (y - iU/4)^2} + s * \ln \frac{1+\eta_1'}{1+\eta_1}\bigg|_{\sin k}$$

$$\ln \eta_n = s * \ln\left((1+\eta_{n-1})(1+\eta_{n+1})\right) - \delta_{n1} s * \ln\left(1+\zeta^{-1}\right), \quad \eta_0(\Lambda) = \eta_0'(\Lambda) = 0$$

$$\ln \eta_n' = s * \ln\left((1+\eta_{n-1}')(1+\eta_{n+1}')\right) - \delta_{n1} s * \ln(1+\zeta), \quad n \in \mathbb{N}$$

- kernel s and boundary conditions are

$$s(x) = \frac{1}{U \cosh\left(\frac{2\pi}{U} x\right)},$$

$$\lim_{n\to\infty} \frac{\eta_n(\Lambda)}{n} = 2\beta B, \qquad \lim_{n\to\infty} \frac{\ln \eta_n'(\Lambda)}{n} = -2\beta\mu$$

TBA for Hubbard: Free Energy

The host's part of the thermodynamical potential

$$f_{\mathsf{h}} = \frac{U}{4} - T\int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \ln\left(1 + \frac{1}{\zeta(k)}\right) - T\sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \frac{\mathrm{d}\Lambda}{\pi} \ln\left(1 + \frac{1}{\eta_n'(\Lambda)}\right) \mathsf{Re}\frac{1}{\sqrt{1-\left(\Lambda - in\frac{U}{4}\right)^2}}.$$

The impurity part

$$f_i = \frac{U}{4} - T\int_{-\pi}^{\pi} \mathrm{d}k\hat{\Delta}(k) \ln\left(1 + \frac{1}{\zeta(k)}\right)$$
$$-\frac{4T}{\pi}\sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\Lambda \left(\partial_\Lambda \hat{\delta}\left(\mathsf{Re}\frac{1}{\sqrt{1-\left(\Lambda - ni\frac{U}{4}\right)^2}}\right)\right) \ln\left(1 + \frac{1}{\eta_n'(\Lambda)}\right).$$

Continuum limit of TBA - Anderson Impurity Model

- Continuum limit yields

$$\ln \overline{\zeta}(k) = \beta(k - \epsilon_d - \overline{U}/2) - \int_{\mathbb{R}} \mathrm{d}p R\left(g\left(k\right) - g\left(p\right)\right) p g'(p) + T\, \overline{s} * \ln \frac{1 + \overline{\eta}'_1}{1 + \overline{\eta}_1}\Big|_{g(k)}$$

$$\ln \overline{\eta}_n = \overline{s} * \ln\left[\left(1 + \overline{\eta}_{n-1}\right)\left(1 + \overline{\eta}_{n+1}\right)\right] - \delta_{n1} \overline{s} * \ln\left(1 + \overline{\zeta}^{\,-1}\right)$$

$$\ln \overline{\eta}'_n = \overline{s} * \ln\left[\left(1 + \overline{\eta}'_{n-1}\right)\left(1 + \overline{\eta}'_{n+1}\right)\right] - \delta_{n1} \overline{s} * \ln\left(1 + \overline{\zeta}\right)$$

- with kernels

$$\overline{s}\left(x\right) = \frac{1}{2\cosh(\pi x)}, \quad R\left(x\right) = \int_0^\infty \frac{\mathrm{d}\omega}{\pi} \frac{\cos\left(\omega x\right)}{1 + e^\omega}, \quad \Delta\left(k\right) = \frac{1}{2\pi \mathrm{i}} \partial_k \log \frac{k - \epsilon_d - i\frac{\bar{V}^2}{2}}{k - \epsilon_d + i\frac{\bar{V}^2}{2}}$$

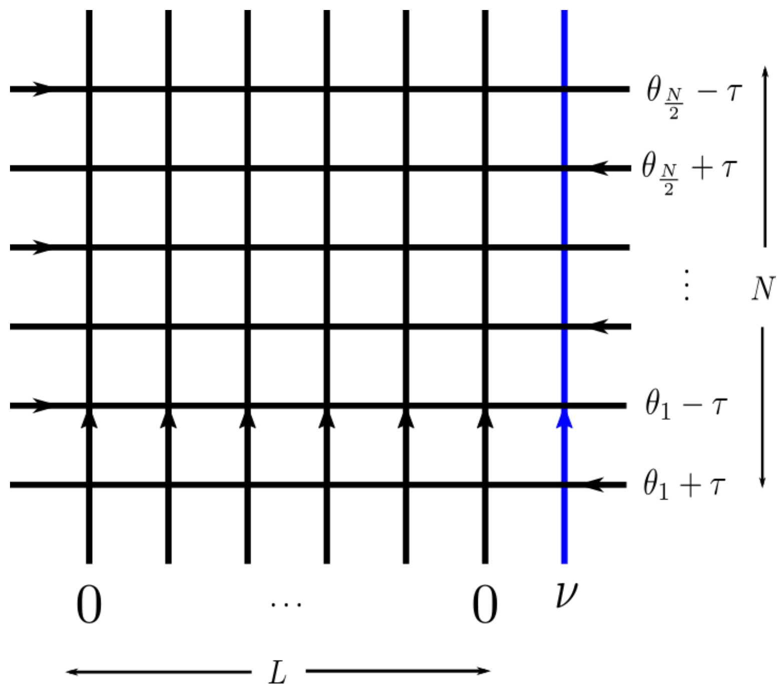
- free energies

$$f_h = -\frac{T}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k \ln\left(1 + \bar{\zeta}^{-1}\right) - \frac{T}{2\pi} \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}k \int_{-\infty}^{\infty} \mathrm{d}\lambda a_n\left(\lambda - g\left(k\right)\right) \ln\left(1 + \bar{\eta}'^{-1}_n\left(\lambda\right)\right)$$

$$f_i = -T \int_{-\infty}^{\infty} \mathrm{d}k \ln\left(1 + \bar{\zeta}^{-1}\right) \Delta\left(k\right) - T \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}k \int_{-\infty}^{\infty} \mathrm{d}\lambda \Delta\left(k\right) a_n\left(\lambda - g\left(k\right)\right) \ln\left(1 + \bar{\eta}'^{-1}_n\left(\lambda\right)\right)$$

Thermodynamics by Use of the Quantum Transfer Matrix

Two-dimensional classical model onto which the quantum chain at finite temperature is mapped



Alternating rows of the lattice correspond to $\exp(-2\tau H_\theta)$, $\tau = \beta/N$

Free energy from just the largest eigenvalue of the column-to-column transfer matrix (quantum transfer matrix).

The blue line corresponds to the impurity.

Finite Set of Non-linear Integral Equations: Hubbard

Alternative description by use of 6 auxiliary functions

$$\ln \mathfrak{b}^{+} = -2\beta B - K_2 * \ln \mathfrak{B}^{+} + K_{2,\frac{U}{2}} * \ln \mathfrak{B}^{-} - K_1 * \ln \frac{\bar{\mathfrak{c}}^{+}\bar{\mathfrak{C}}^{-}}{\bar{\mathfrak{c}}^{-}\bar{\mathfrak{C}}^{+}}$$

$$\ln \mathfrak{b}^{-} = -2\beta B - K_{2,-\frac{U}{2}} * \ln \mathfrak{B}^{+} + K_2 * \ln \mathfrak{B}^{-} - K_{1,-\frac{U}{2}} * \ln \frac{\bar{\mathfrak{c}}^{+}\bar{\mathfrak{C}}^{-}}{\bar{\mathfrak{c}}^{-}\bar{\mathfrak{C}}^{+}}$$

$$\ln \mathfrak{c}^{\pm} = -\frac{\beta U}{2} + \beta\left(\mu + B\right) \pm 2\beta\sqrt{1-s^2} - K_1 * \ln \bar{\mathfrak{B}}^{-} + K_{1,-\frac{U}{4}} * \ln \frac{\bar{\mathfrak{C}}^{+}}{\bar{\mathfrak{C}}^{-}} \pm \frac{1}{2} \ln \frac{\bar{\mathfrak{C}}^{+}}{\bar{\mathfrak{C}}^{-}},$$

$$\ln \bar{\mathfrak{c}}^{\pm} = -\frac{\beta U}{2} - \beta\left(\mu + B\right) \mp 2\beta\sqrt{1-s^2} + K_{1,\frac{U}{2}} * \ln \mathfrak{B}^{-} - K_{1,\frac{U}{4}} * \ln \frac{\mathfrak{C}^{+}}{\mathfrak{C}^{-}} \pm \frac{1}{2} \ln \frac{\mathfrak{C}^{+}}{\mathfrak{C}^{-}}.$$

The host's contribution to the free energy

$$f_{\mathsf{h}} = \frac{U}{4} - \frac{1}{\beta}\int_{\mathcal{L}} \mathrm{d}s \left[\ln z\left(s - i\frac{U}{2}\right)\right]' \ln \mathfrak{C}\left(s\right) - \frac{1}{\beta}\int_{\mathcal{L}} \mathrm{d}s \left[\ln z\left(s\right)\right]' \ln \frac{1+\mathfrak{c}+\bar{\mathfrak{c}}}{\bar{\mathfrak{c}}}\left(s\right).$$

Finite NLIE – Hubbard: Free Energy of Host and Impurity

The host's contribution to the free energy

$$f_{\mathsf{h}} = \frac{U}{4} - \frac{1}{\beta} \int\limits_{\mathcal{L}} \mathrm{d}s \left[\ln z \left(s - i\frac{U}{2} \right) \right]' \ln \mathfrak{C}(s) - \frac{1}{\beta} \int\limits_{\mathcal{L}} \mathrm{d}s \left[\ln z(s) \right]' \ln \frac{1 + \mathfrak{c} + \bar{\mathfrak{c}}}{\bar{\mathfrak{c}}}(s) \, .$$

Impurity

$$\begin{aligned} -\beta f_i = {} & \left(\frac{1}{2 z_+(x)} - \frac{z_-(x)}{2} - \frac{U}{4} + \mu \right) \beta + \ln \left(e^{\beta B} + e^{\beta \mu} + e^{-\beta \mu} + e^{-\beta B} \right) \\ & - \frac{1}{2\pi i} \left(k \circ \ln \mathfrak{B} \right)(s) + \frac{1}{2\pi i} \left(k \circ \left(\ln \bar{\mathfrak{C}} - \ln \bar{\mathfrak{c}} - \ln \mathfrak{B} \right) \right) \left(s - i\frac{U}{2} \right) \\ & + \int\limits_{\mathcal{L}} \frac{\mathrm{d}s'}{2\pi i} \left[\ln g \left(s' - i\frac{U}{2} \right) \right]' \ln \mathfrak{C}(s') + \int\limits_{\mathcal{L}} \frac{\mathrm{d}s'}{2\pi i} \left[\ln g(s') \right]' \ln \frac{1 + \mathfrak{c} + \bar{\mathfrak{c}}}{\bar{\mathfrak{c}}}(s') \\ & + \int\limits_{\mathcal{L}} \frac{\mathrm{d}s'}{2\pi i} \ln \left(\left(1 - z_-^2(x) + 2 i z_-(x) s' \right) \left(1 - z_+^2(x) + 2 i z_+(x) s' \right) \right) \left[\ln \left(\frac{1 + \mathfrak{c} + \bar{\mathfrak{c}}}{\bar{\mathfrak{c}}} \frac{\bar{\mathfrak{c}} \mathfrak{B}}{1 + \bar{\mathfrak{c}} \mathfrak{B}} \right)(s') \right]' \end{aligned}$$

Continuum limit of NLIE - Anderson Impurity Model

$$\ln \mathfrak{b}^{+} = -\beta H - \mathcal{K}_{4,0} * \ln \mathfrak{B}^{+} + \mathcal{K}_{4,1} * \ln \mathfrak{B}^{-} - \mathcal{K}_{2,0} * \ln \frac{\bar{\mathfrak{c}}^{+}}{\bar{\mathfrak{C}}^{+}},$$

$$\ln \mathfrak{b}^{-} = -\beta H - \mathcal{K}_{4,-\frac{1}{2}} * \ln \mathfrak{B}^{+} + \mathcal{K}_{4,0} * \ln \mathfrak{B}^{-} - \mathcal{K}_{2,-\frac{1}{2}} * \ln \frac{\bar{\mathfrak{c}}^{+}}{\bar{\mathfrak{C}}^{+}},$$

$$\ln \mathfrak{c}\,(k) = \frac{5\beta}{4}\left(H - 2\epsilon_d - \tilde{U}\right) + \mathcal{K}_{4,-\frac{1}{2}} * \ln \mathfrak{B}^{+}\Big|_{g(k)} - \mathcal{K}_{2,1} * \ln \mathfrak{B}^{-}\Big|_{g(k)} + \mathcal{K}_{2,-1} * \ln \bar{\mathfrak{B}}^{+}\Big|_{g(k)}$$

$$- \mathcal{K}_{2,0} * \ln \bar{\mathfrak{B}}^{-}\Big|_{g(k)} + \mathcal{K}_{4,0} * \ln \mathfrak{C} + \mathcal{K}_{2,-\frac{1}{2}} * \ln \bar{\mathfrak{C}} + \frac{1}{2} \ln \bar{\mathfrak{C}},$$

$$\ln \bar{\mathfrak{c}}\,(k) = -\frac{\beta}{2}\,(H - k) - \mathcal{K}_{2,0} * \ln \mathfrak{B}^{+}\Big|_{g(k)} + \mathcal{K}_{2,1} * \ln \mathfrak{B}^{-}\Big|_{g(k)} - \mathcal{K}_{2,\frac{1}{2}} * \ln \mathfrak{C} + \frac{1}{2} \ln \mathfrak{C}$$

$$\bar{s} = -1 + \frac{U}{8V^2} - \frac{V^2}{8U}$$

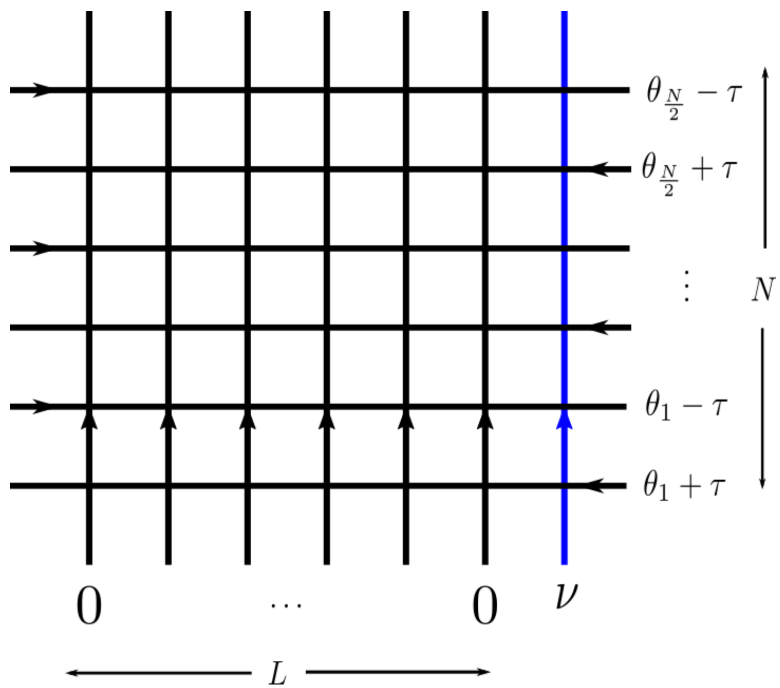
$$-\beta f_h = \int_{\mathcal{L}} \frac{\mathrm{d}s}{2\pi \mathrm{i}} \frac{1}{\sqrt{s^2 - 1}} \ln \mathfrak{C}\,(s) + \int_{\mathcal{L}} \frac{\mathrm{d}s}{2\pi \mathrm{i}} \frac{1}{\sqrt{s^2 - 1}} \ln \frac{1 + \mathfrak{c} + \bar{\mathfrak{c}}}{\bar{\mathfrak{c}}}\,(s)$$

$$-\beta f_i = -\beta(2\epsilon_d + \bar{U}) + \ln\left(e^{\beta H/2} + e^{\beta\left(2\epsilon_d + \bar{U}\right)} + e^{-\beta\left(2\epsilon_d + \bar{U}\right)} + e^{-\beta H/2)}\right)$$

$$+ k \circ \left(\ln \frac{\bar{\mathfrak{C}}}{\bar{\mathfrak{c}}} + \ln \frac{1 + \mathfrak{c} + \bar{\mathfrak{c}}}{1 + \bar{\mathfrak{c}}\mathfrak{B}}\right)(\bar{s}) + \int_{\mathcal{L}} \frac{\mathrm{d}s}{2\pi \mathrm{i}} \left[\ln \frac{(z\,(s) - 1)^2}{z\,(s)}\right]' \left(\ln \mathfrak{C} + \ln \frac{1 + \mathfrak{c} + \bar{\mathfrak{c}}}{\bar{\mathfrak{c}}}\right)(s)$$

Modification of Hamiltonians by Shifts of Spectral Parameters

Again: two-dimensional classical model $\equiv$ quantum chain at finite temperature



Alternating rows of the lattice correspond to $\exp(-2\tau H_\theta)$, $\tau = \beta/N$

Now use some non-zero values for the $\theta' s$. Use distribution function

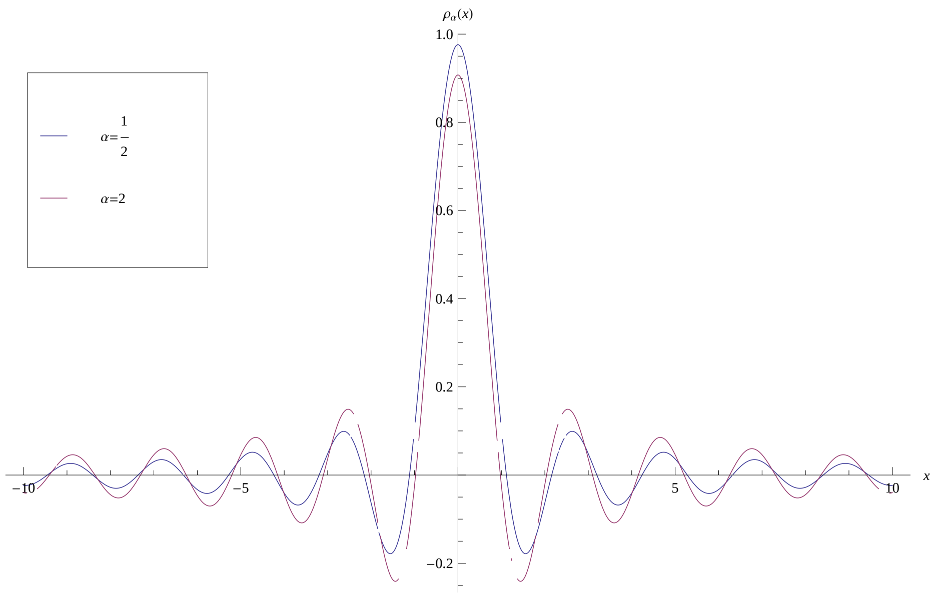
$$\rho_\alpha(s) = \frac{\alpha\Gamma\left(\frac{\alpha}{2}\right)}{2\sqrt{\pi}\Gamma\left(\frac{3+\alpha}{2}\right)} \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{4\pi} e^{iks} |k| \frac{{}_0F_1\left(;\frac{3+\alpha}{2};-\frac{k^2}{4}\right)}{J_1(|k|)},$$

Modifications: Distribution of Shifts of Spectral Parameters

The distribution function

$$\rho_\alpha\left(s\right)=\frac{\alpha\Gamma\left(\frac{\alpha}{2}\right)}{2\sqrt{\pi}\Gamma\left(\frac{3+\alpha}{2}\right)}\int\limits_{-\infty}^{\infty}\frac{\mathrm{d}k}{4\pi}e^{iks}\left|k\right|\frac{{}_0F_1\left(;\frac{3+\alpha}{2};-\frac{k^2}{4}\right)}{J_1\left(\left|k\right|\right)},$$

is not strictly positive



Negative values of $\rho_{\alpha_h}\left(s\right)$ are associated with the inversion of arrow directions on the lattice.

Modification of Thermodynamics - NLIE (“experimental”)

Most of the thermodynamics expressions remain intact.

- integrals for free energies as written
- coupled non-linear integral equations keep their form, except for replacement

$$e_0(s) \to e_{\text{new}}(s) := (\rho_\alpha * e_0)(s) = \frac{2\sqrt{\pi}\Gamma\left(\frac{3+\alpha}{2}\right)}{\alpha\Gamma\left(\frac{\alpha}{2}\right)}\left(1-s^2\right)^{\frac{\alpha}{2}} \to\sim \left(\frac{k-\epsilon_d-\frac{U}{2}}{\sqrt{U}V}\right)^\alpha$$

- energy-momentum dependence no longer linear, with exponent smaller than 1 $\to$ vanishing density of states
- other effects on Hamiltonian weak: hybridization matrix element looks generic

$$\langle\{d,\uparrow\}|\, H\, |\{k_{\text{in}},\uparrow\}\rangle = \frac{[2-\mathrm{i}\cos(k_{\text{in}})]}{(1+t)^3}\cdot \overline{V}a^{1/2} + O(a^{3/2})$$

Summary

Presented work

- identification of a non-trivial “vanishing interaction limit” of the Hubbard / Shastry model
- the Anderson impurity model established as “transparent impurity”
- derivation of finite set of NLIE for the Anderson impurity model
- modified density of states in AIM

Open problems:

- (numerical) investigation of the thermodynamics
- precise analysis of case with modified density of states