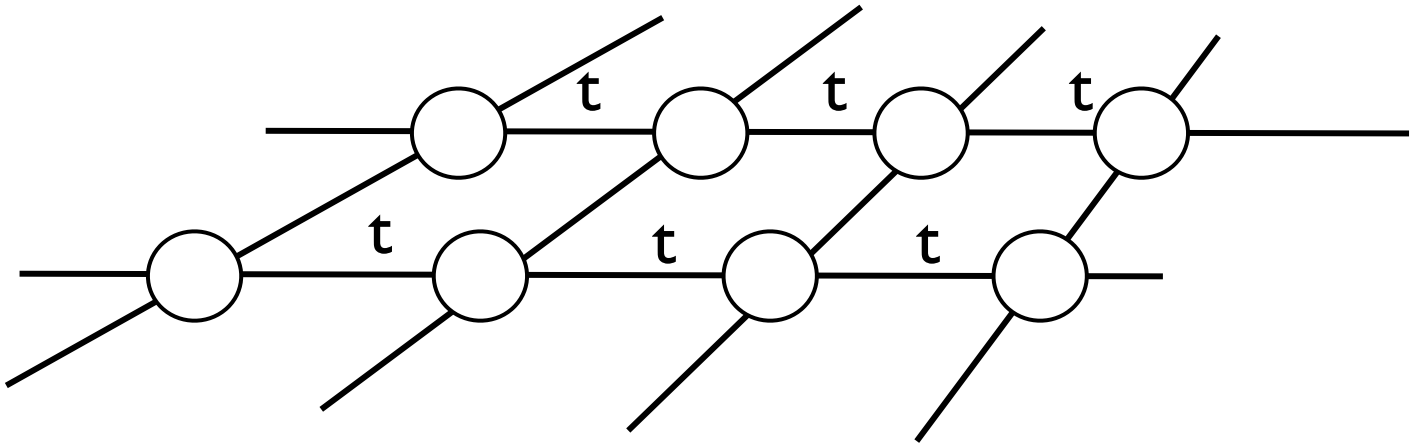
Application of nonlinear canonical transformations to the strong coupling Kondo lattice model

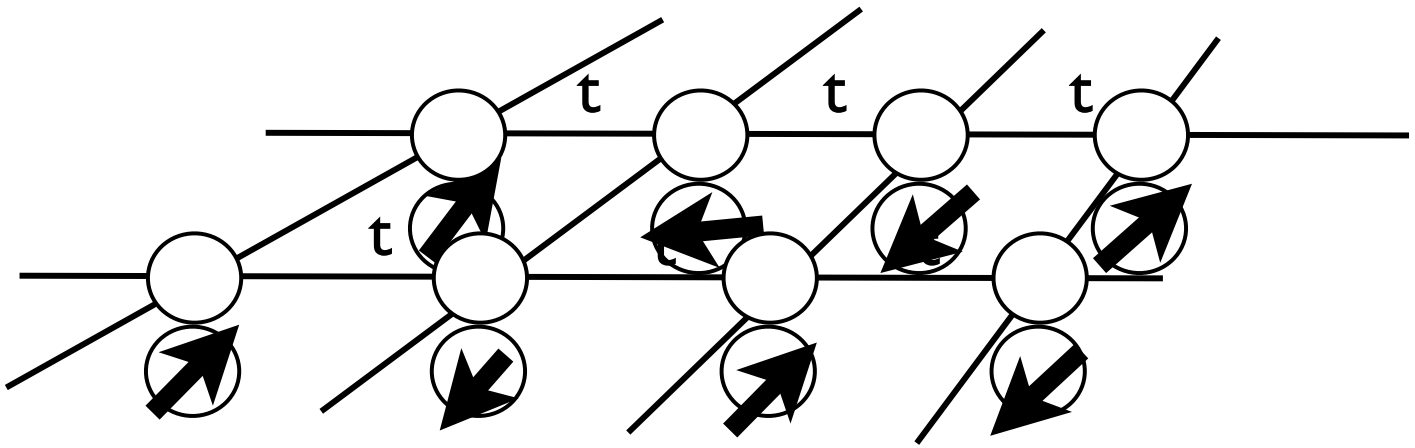
Outline

- Overview of the the Kondo lattice model
- Nonlinear canonical transformation on
  - even valence fermi systems
- Transformations on odd valence insulators

Kondo lattice model: begin with an ordinary tight binding lattice.



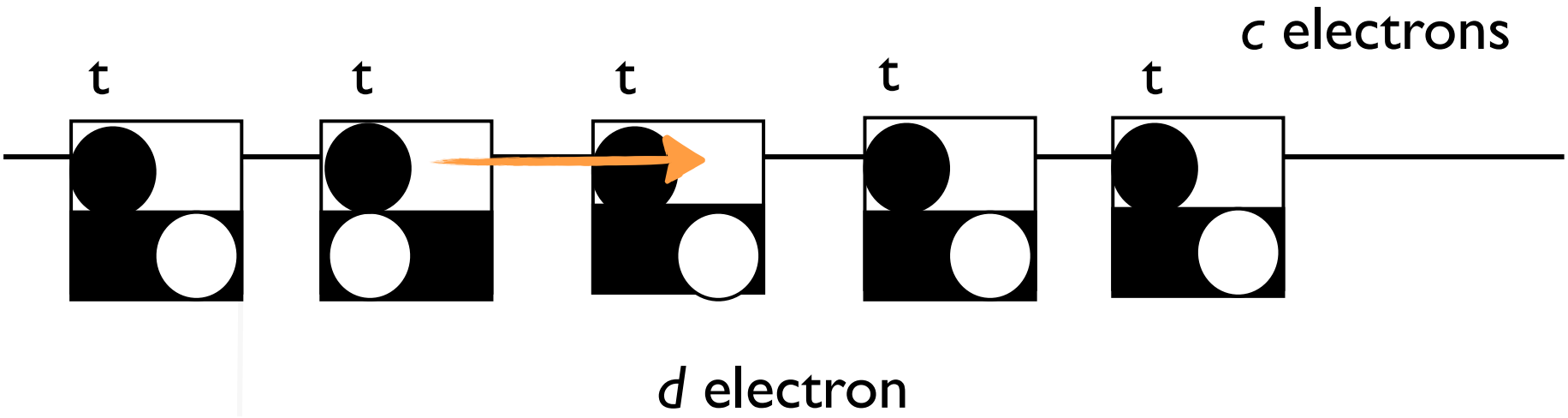
$$-t\sum_{rr'}(c^{\dagger}_{\sigma r}c_{\sigma r}+CC)$$



and layer of deeper localized spins (electrons)

$$H_{Kondo} = \sum_r (JS_r \cdot S_{d,r} + U_d(n_d - 1)^2)$$

Kondo Lattice model:



$$H_{KLM} = -t\sum_{rr'}(c^{\dagger}_{\sigma r}c_{\sigma r} + CC) + \sum_{r}(JS_r \cdot S_{d,r} + U_d(n_d - 1)^2)$$

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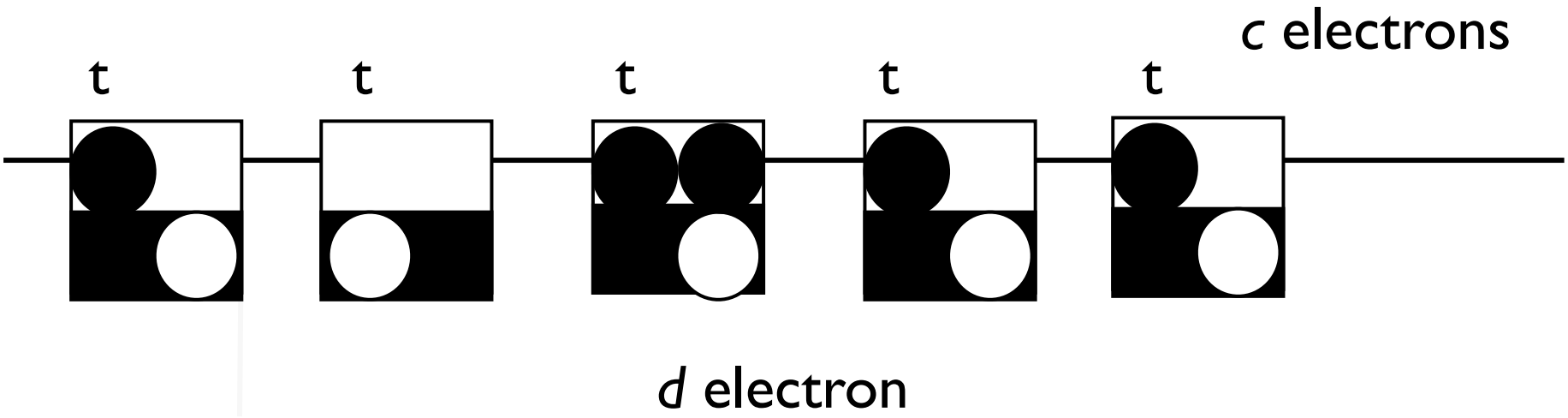

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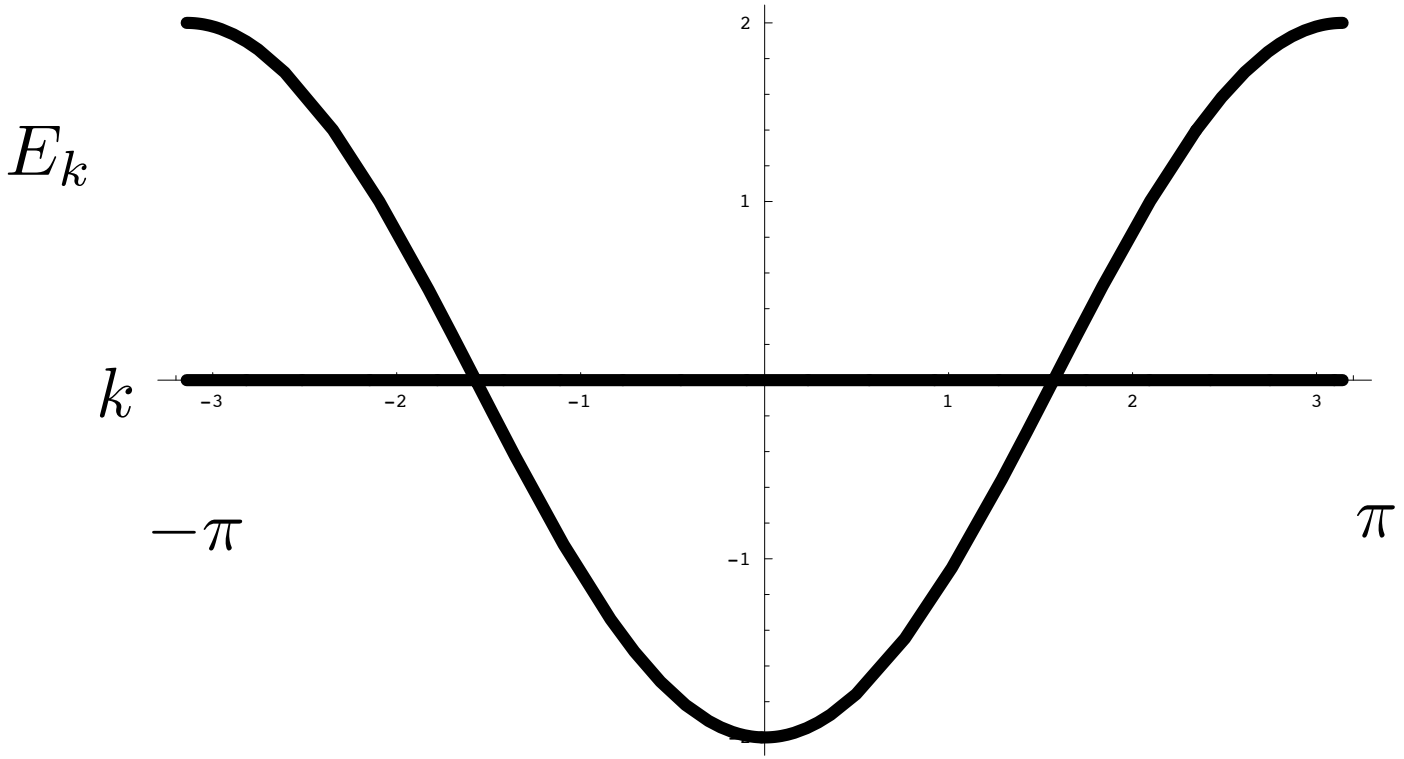
weak coupling J= 0 "RKKY" regime



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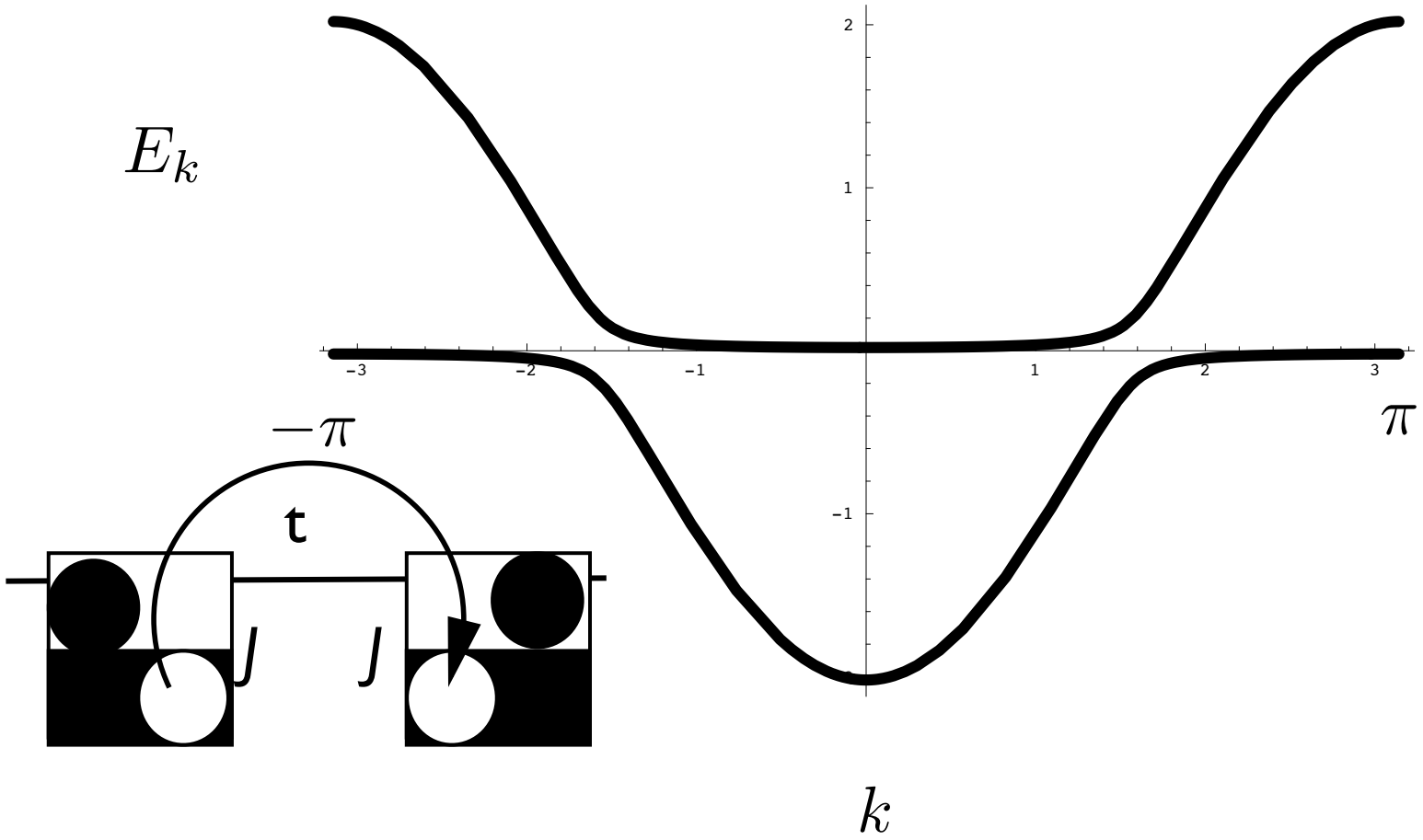
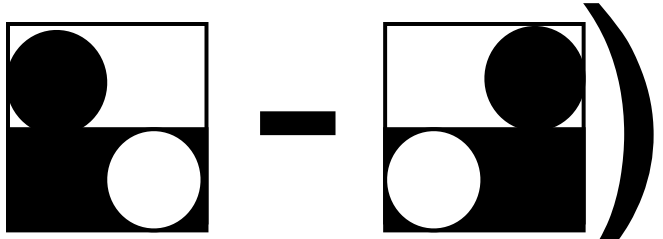
Kondo Lattice model -
weak coupling J ~ 0 "RKKY" regime



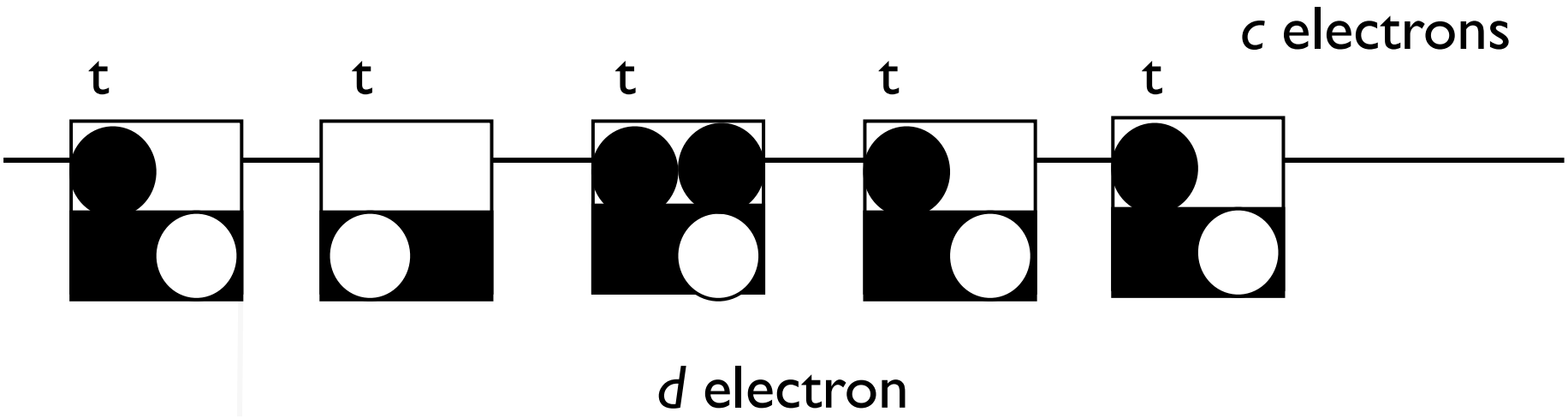
$$H_{int} = \sum_r (JS_r \cdot S_{d,r} + U_d(n_d - 1)^2)$$

Strong coupling limit is very different. $J \gg t$ gives a singlet ground state, with the energy gap of the singly occupied and single vacancy states determining the quasiparticle gap and is an insulator.

$$\frac{1}{\sqrt{2}}\left(\quad - \quad \right)$$

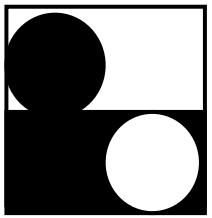
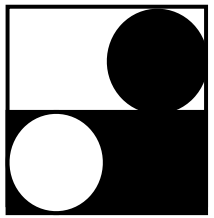


Generalize from Kondo to "Periodic Anderson" models



$$h_{atomic} = \quad \epsilon_d\, n_d + U\, n_{d\uparrow} \cdot n_{d\downarrow} + V\, \Sigma_\sigma (c^\dagger_{0,\sigma} d_\sigma + CC)$$

We look more carefully at the ground state atomic singlet.

$$|\Psi_G\rangle = \frac{1}{\sqrt{2}}\Big($$  $-$  $\Big)$

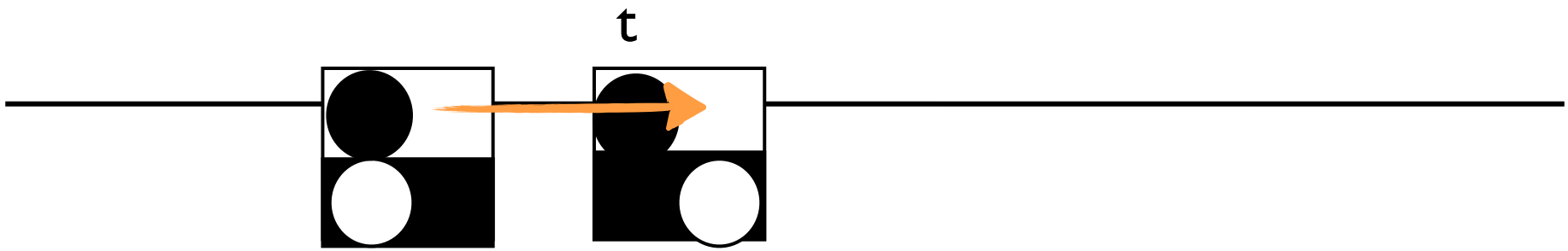
Can we create a local quasiparticle operator which creates an electron or hole on a singlet site?

Quasiparticles require:

A $\hat{c}_\alpha \,|\, \Psi_G \,\rangle = 0$

B $\hat{c}_\alpha \hat{c}_\alpha^\dagger \,|\, \Psi_G \,\rangle = \,|\, \Psi_G \,\rangle$

Do bare electron operators qualify?

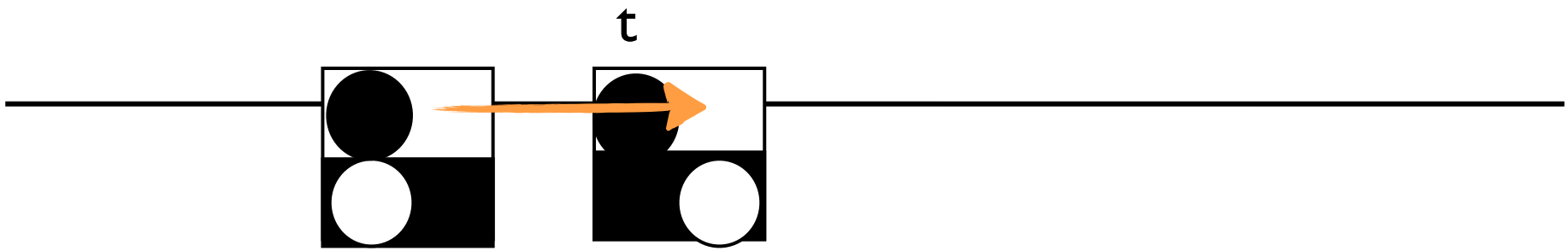


Quasiparticles require:

A $\hat{c}_\alpha \mid \Psi_G \rangle = 0$

$$c_{c,\uparrow} \mid \Psi_G \rangle = \frac{1}{\sqrt{2}} c^\dagger_{f,\downarrow} \mid 0 \rangle \neq 0$$

B $\hat{c}_\alpha \hat{c}^\dagger_\alpha \mid \Psi_G \rangle = \mid \Psi_G \rangle$



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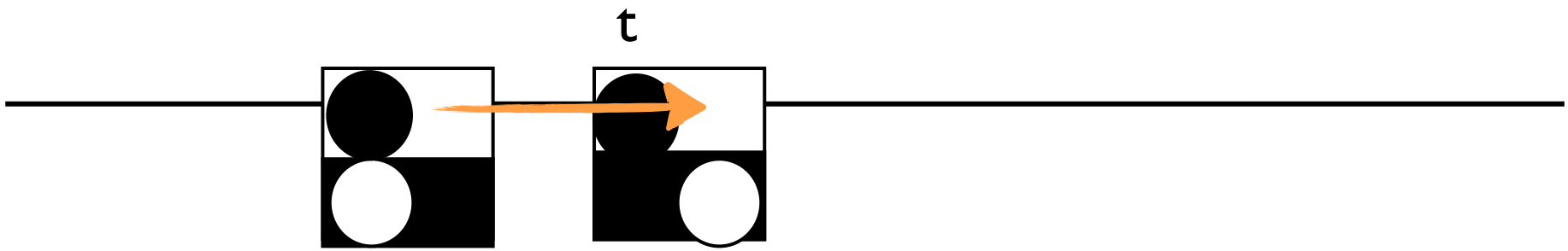

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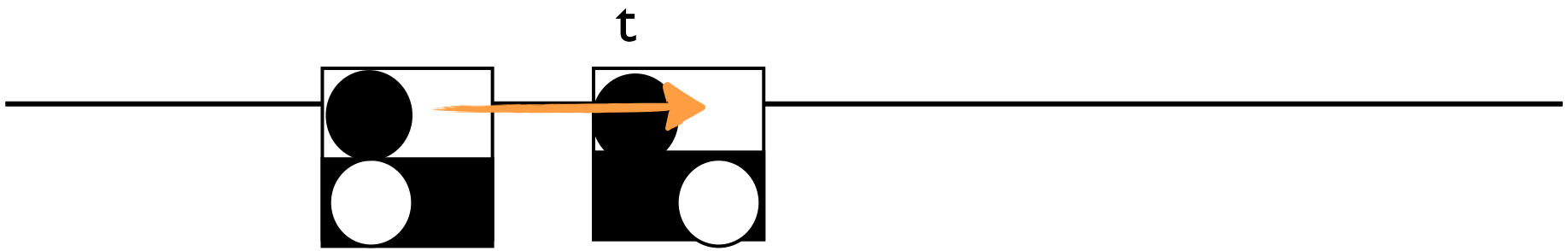

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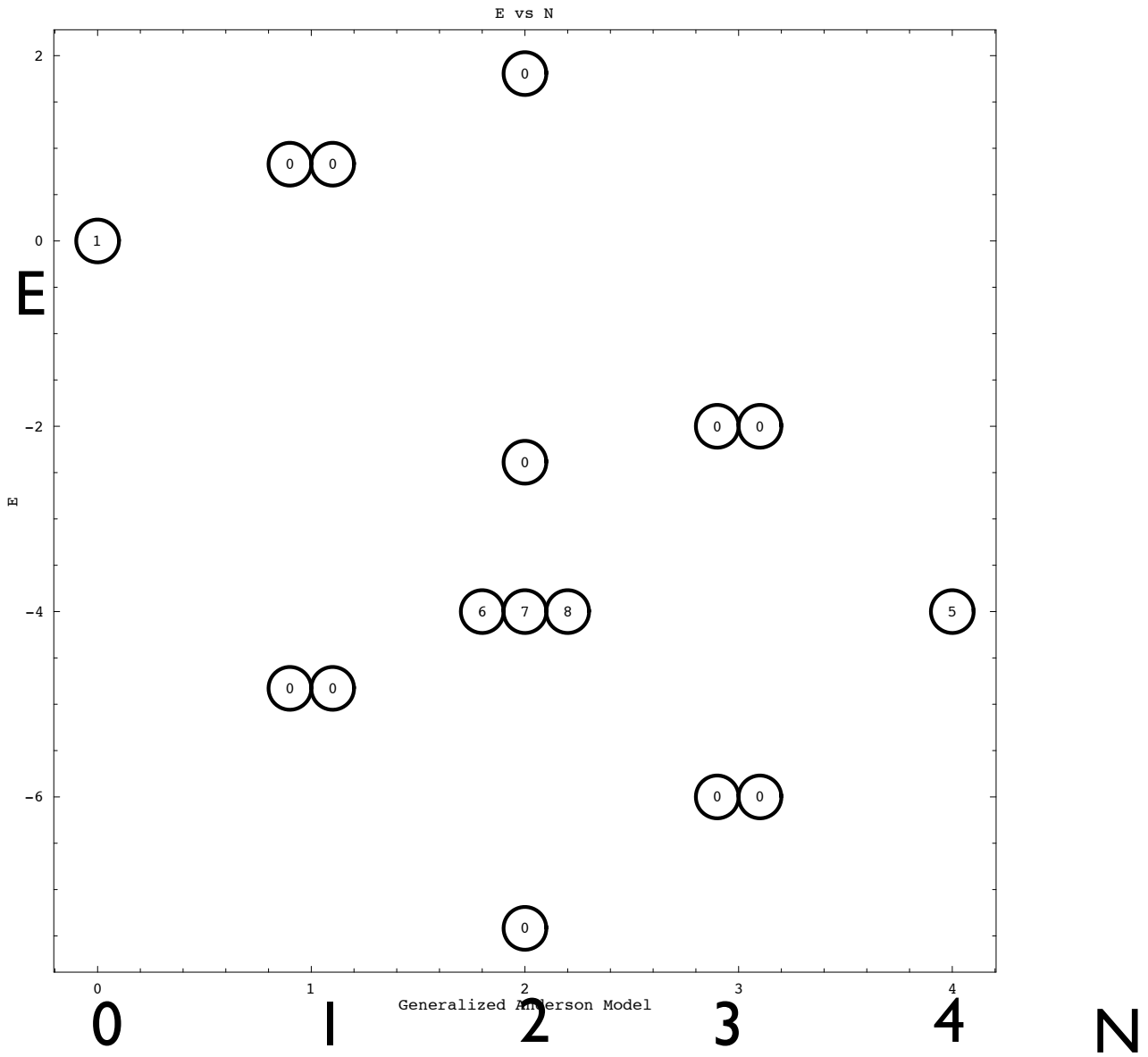
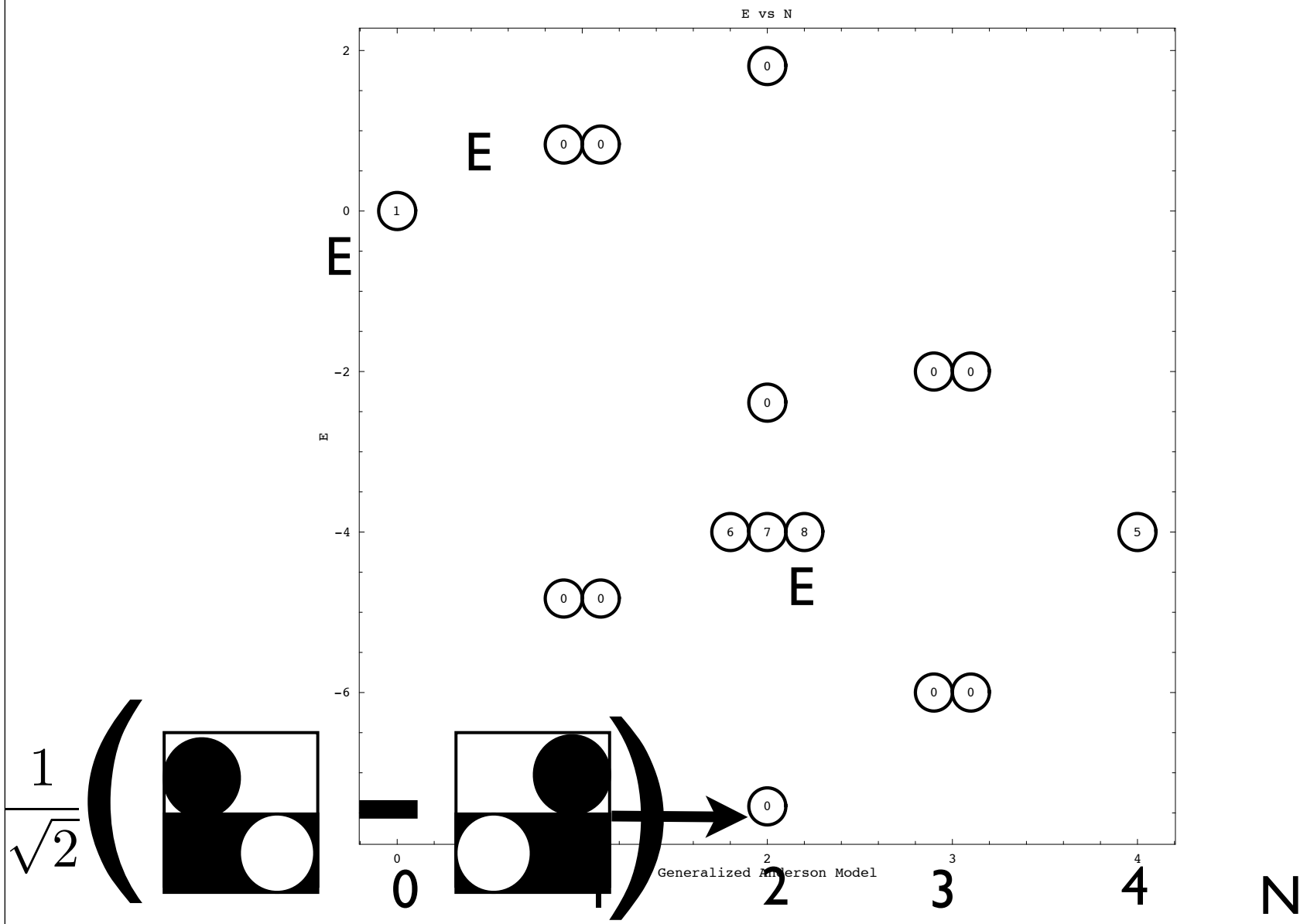
Bare electron operators are no good!

We now turn to dealing with this problem.

We begin by taking a “generic” value of the Anderson impurity parameters and plotting the energy values for different values of the impurity site occupation number.



$$\epsilon_d\, n_d + U\, n_{d\uparrow} \cdot n_{d\downarrow} + V\, \Sigma_\sigma (c^\dagger_{0,\sigma} d_\sigma + CC)$$



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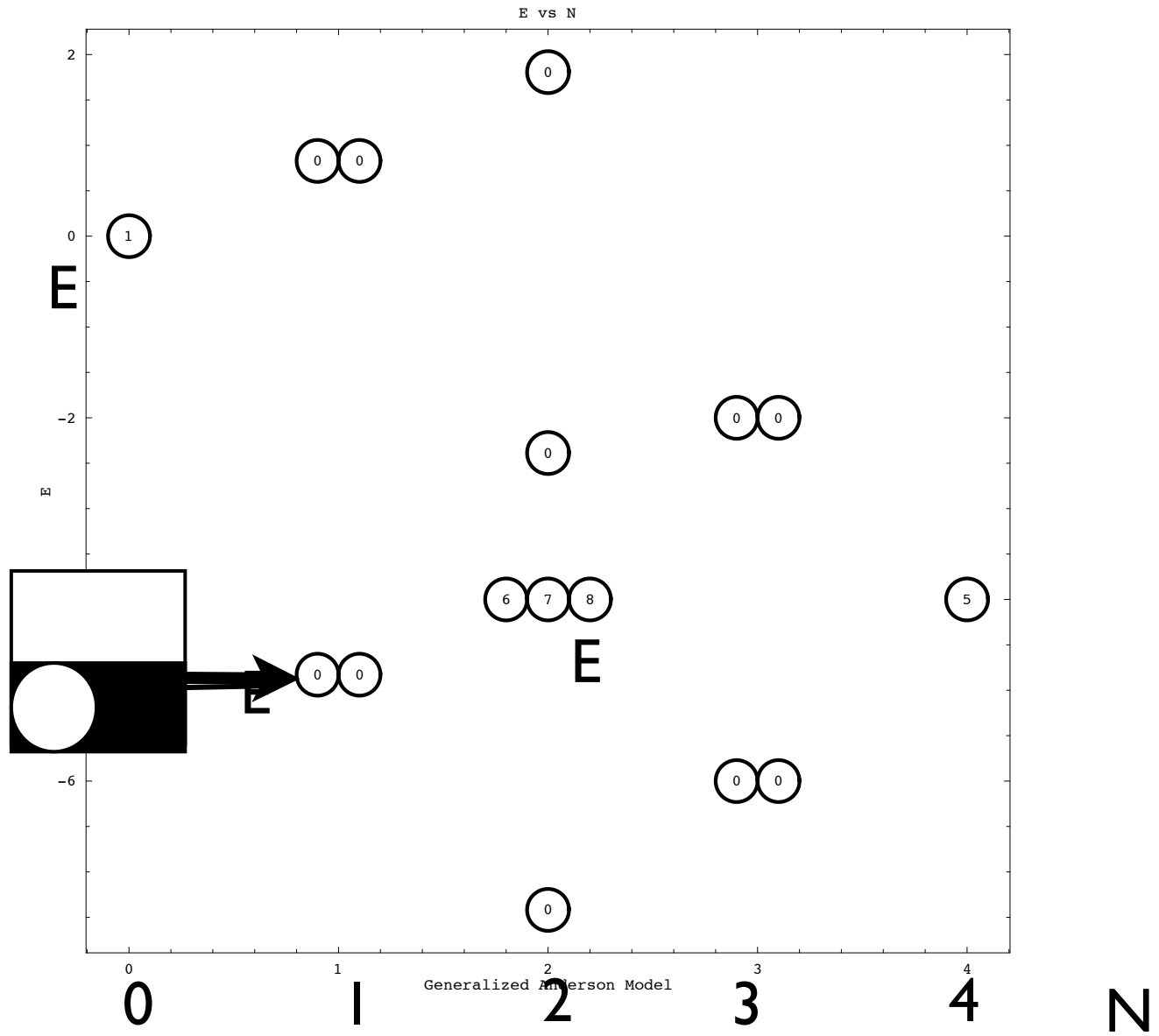

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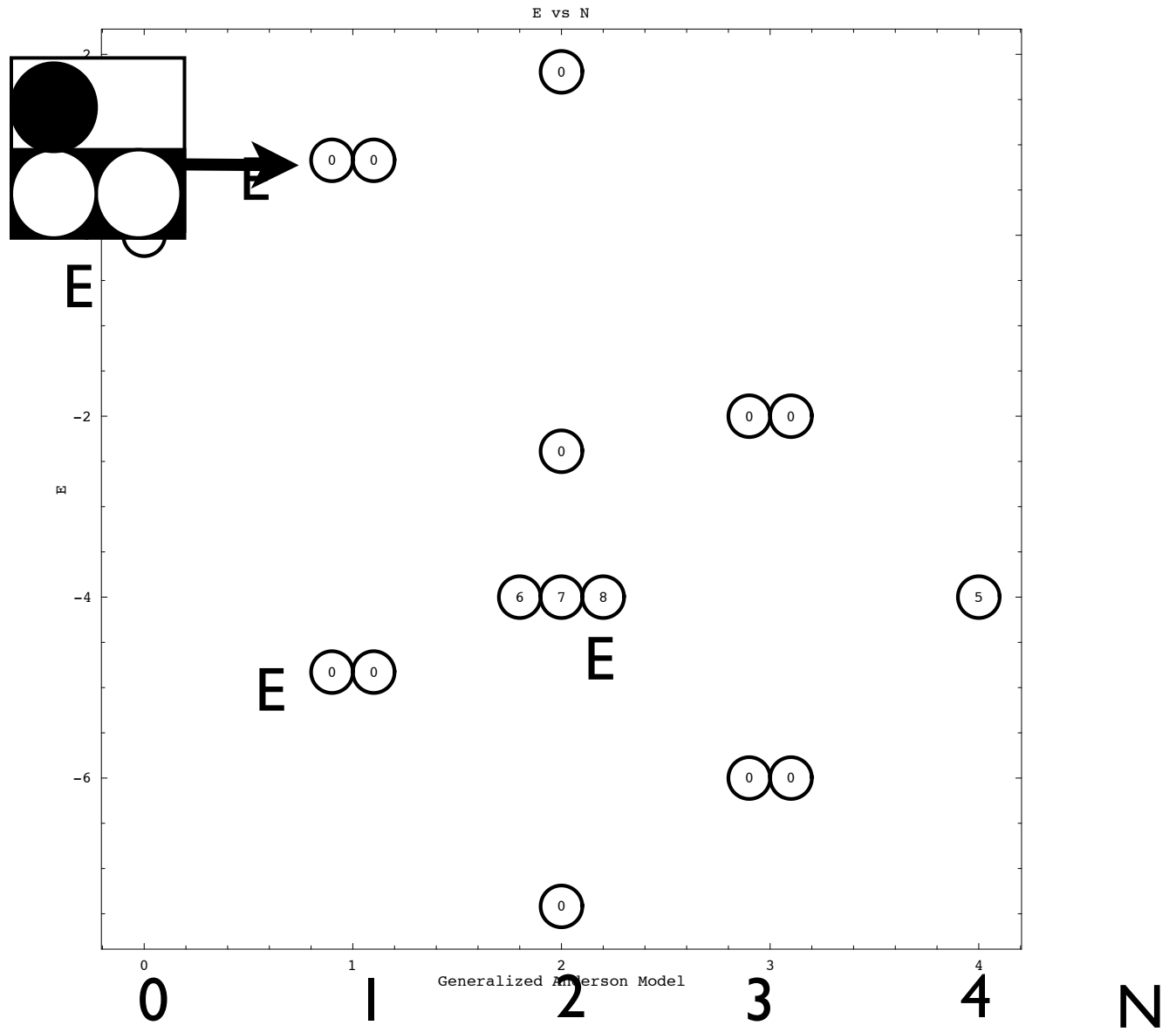

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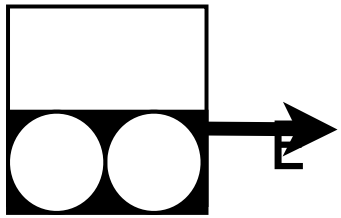

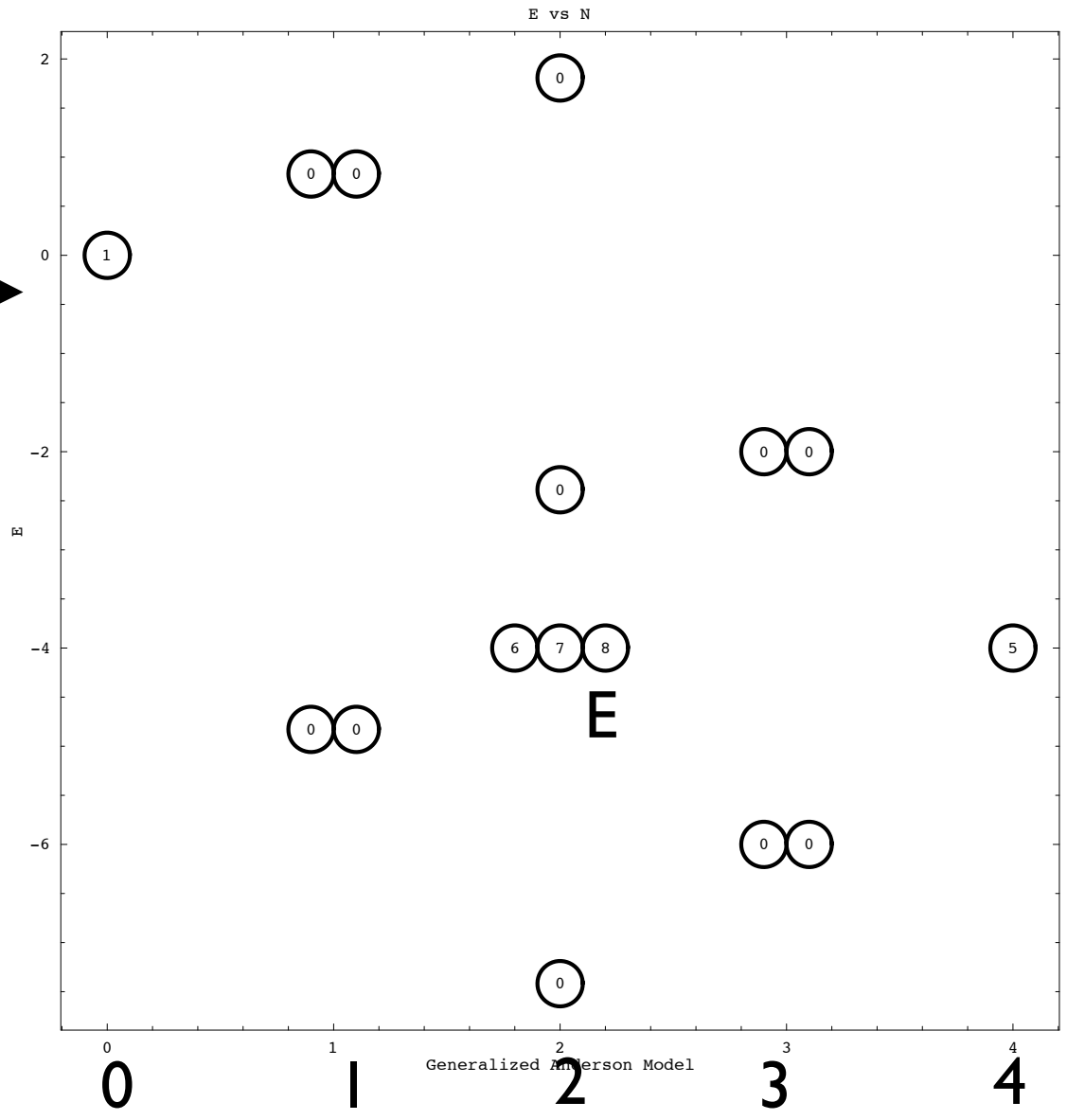

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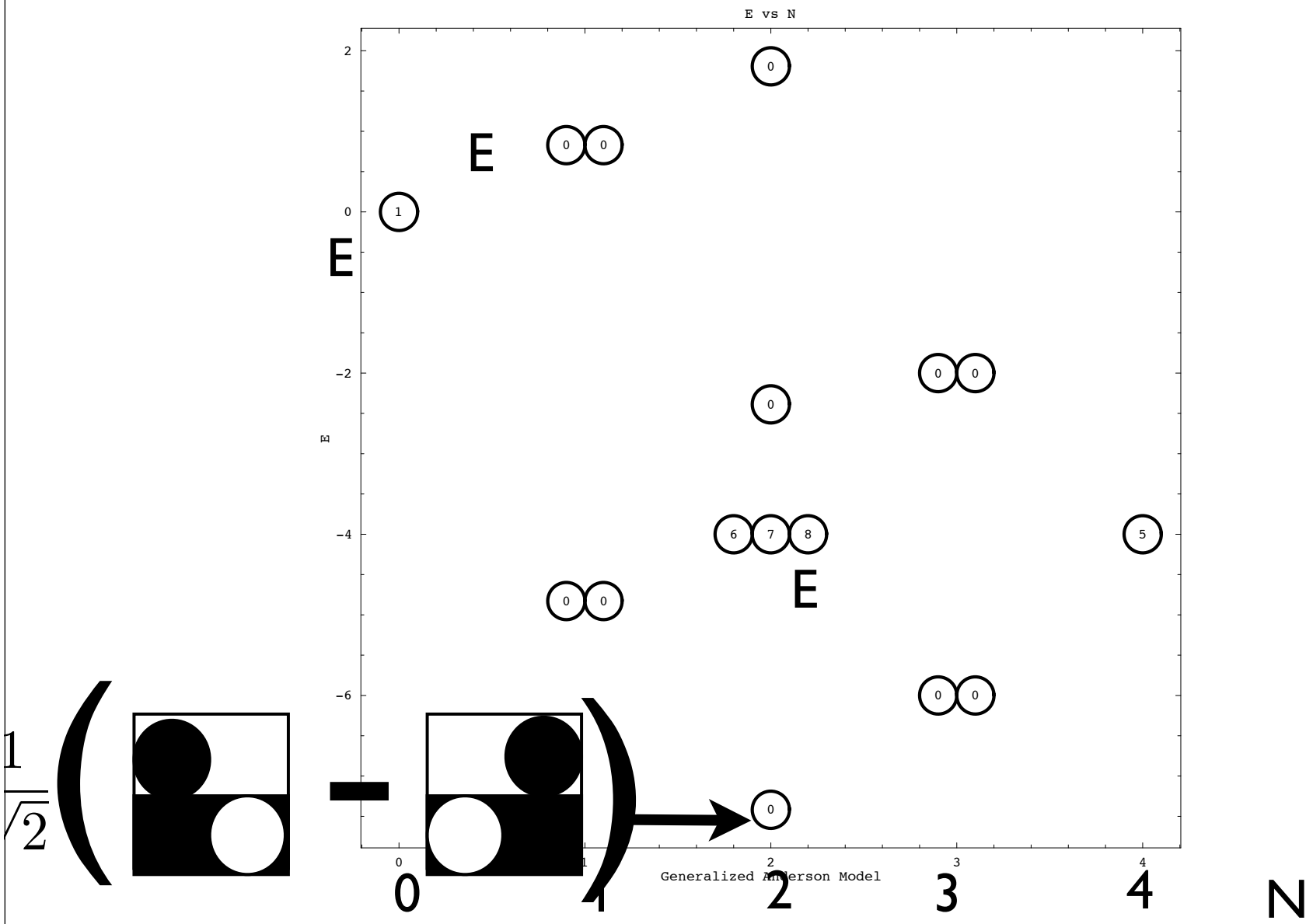

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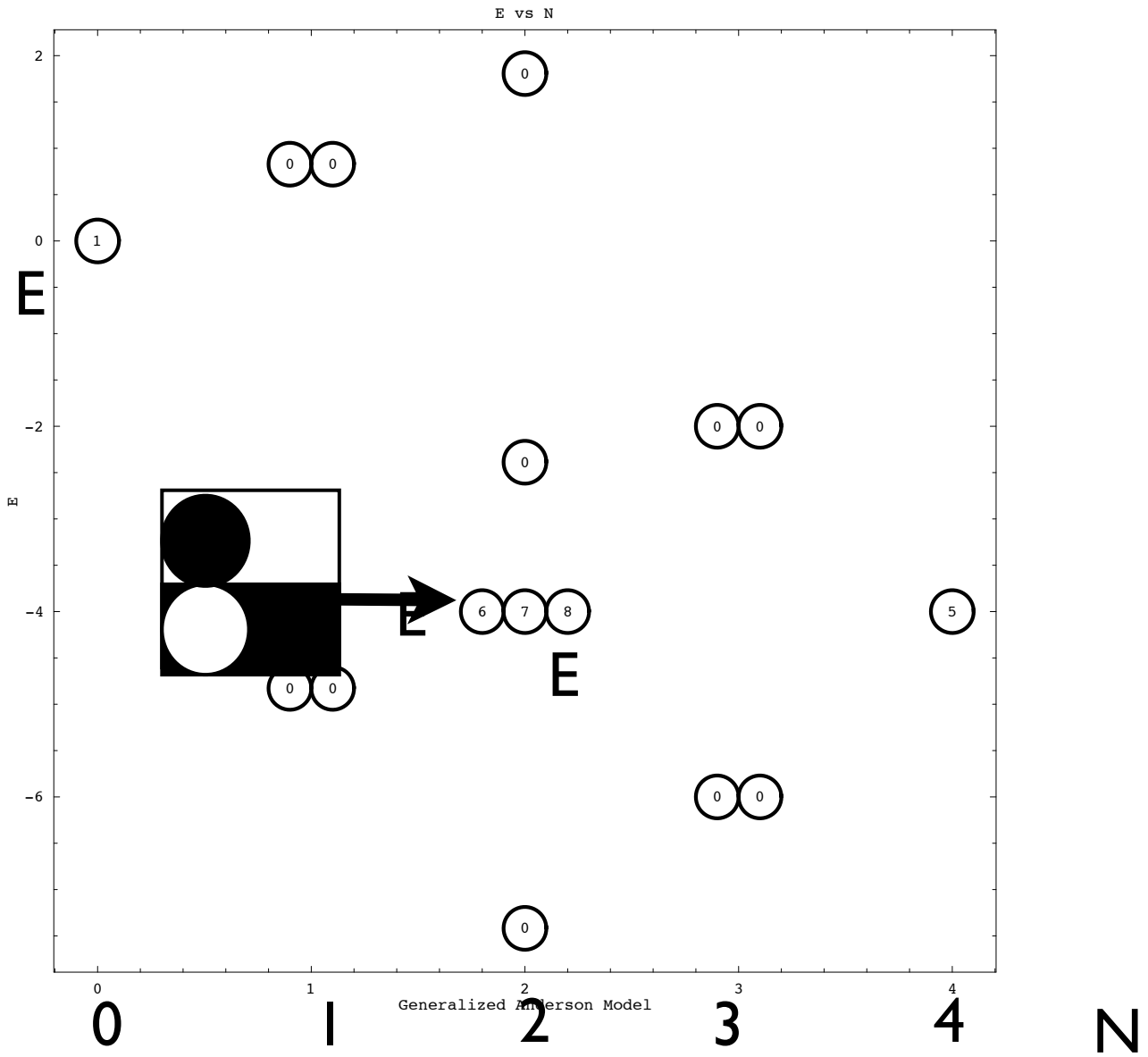

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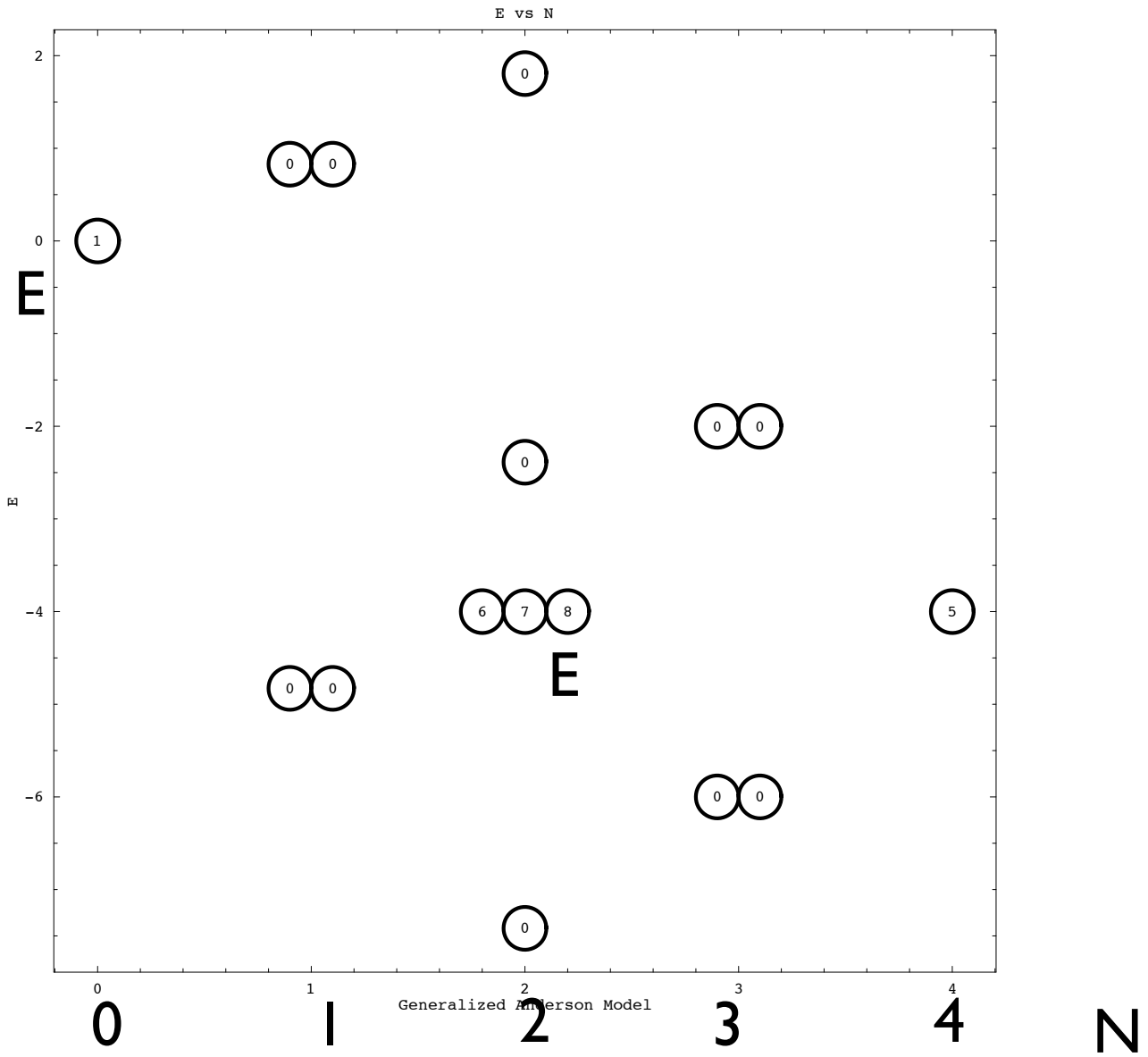
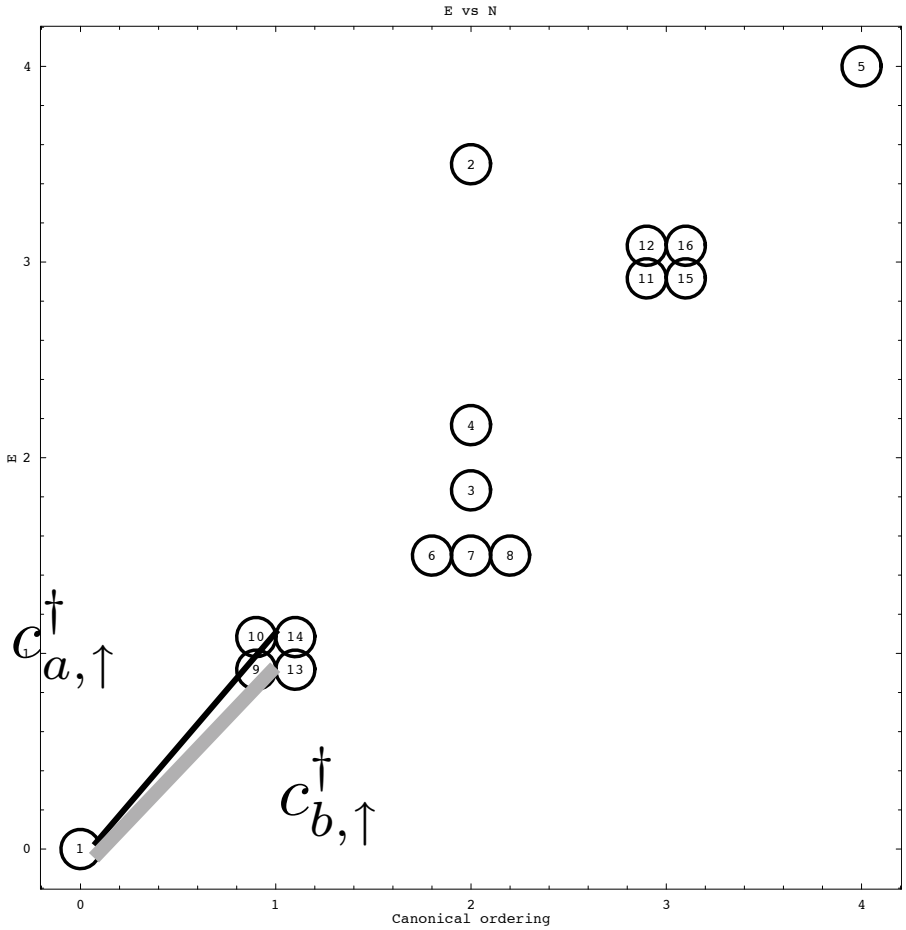


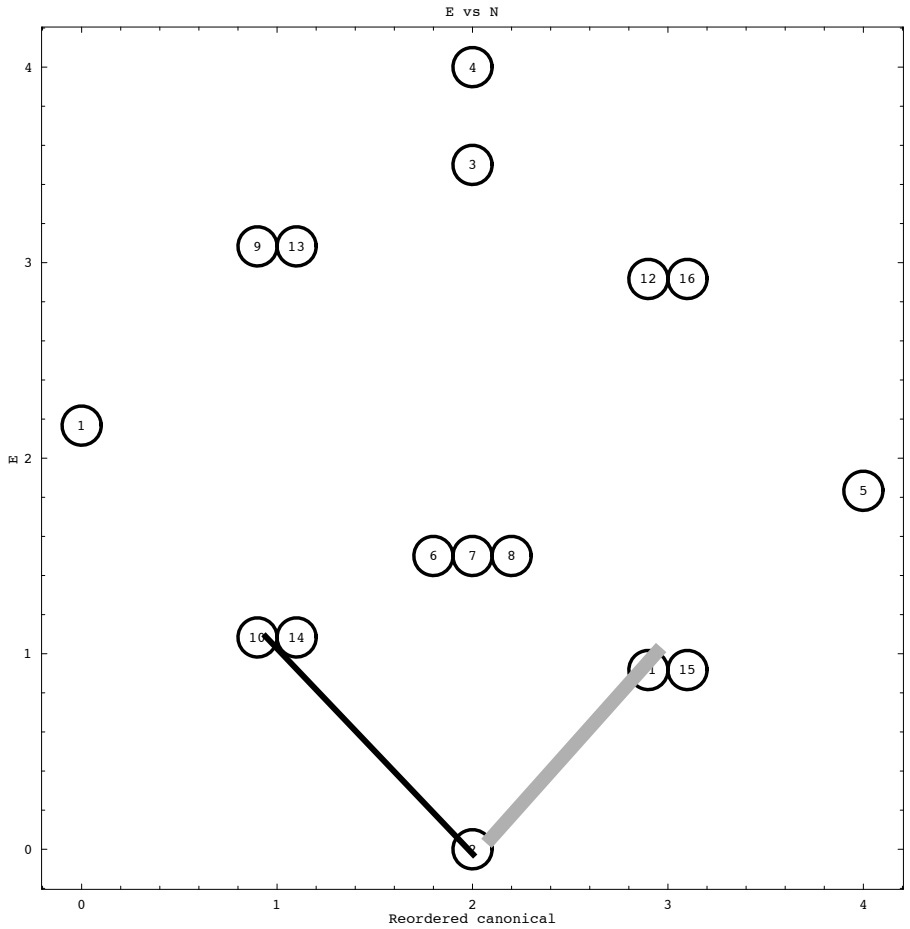
$$\epsilon_d\, n_d + U\, n_{d\uparrow} \cdot n_{d\downarrow} + V\, \Sigma_\sigma (c^\dagger_{0,\sigma} d_\sigma + CC)$$

Another simple Fermi system



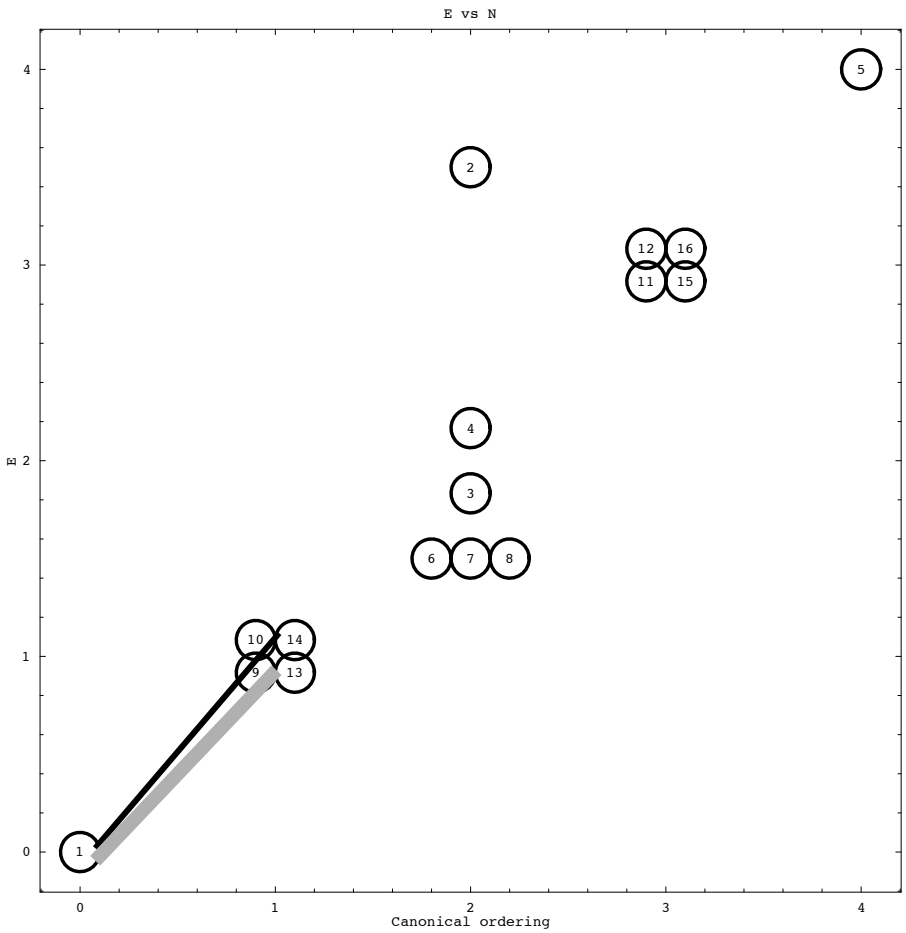
$$n_{tot} + \frac{1}{12}(n_a - n_b) - \frac{1}{2} S_a \cdot S_b$$

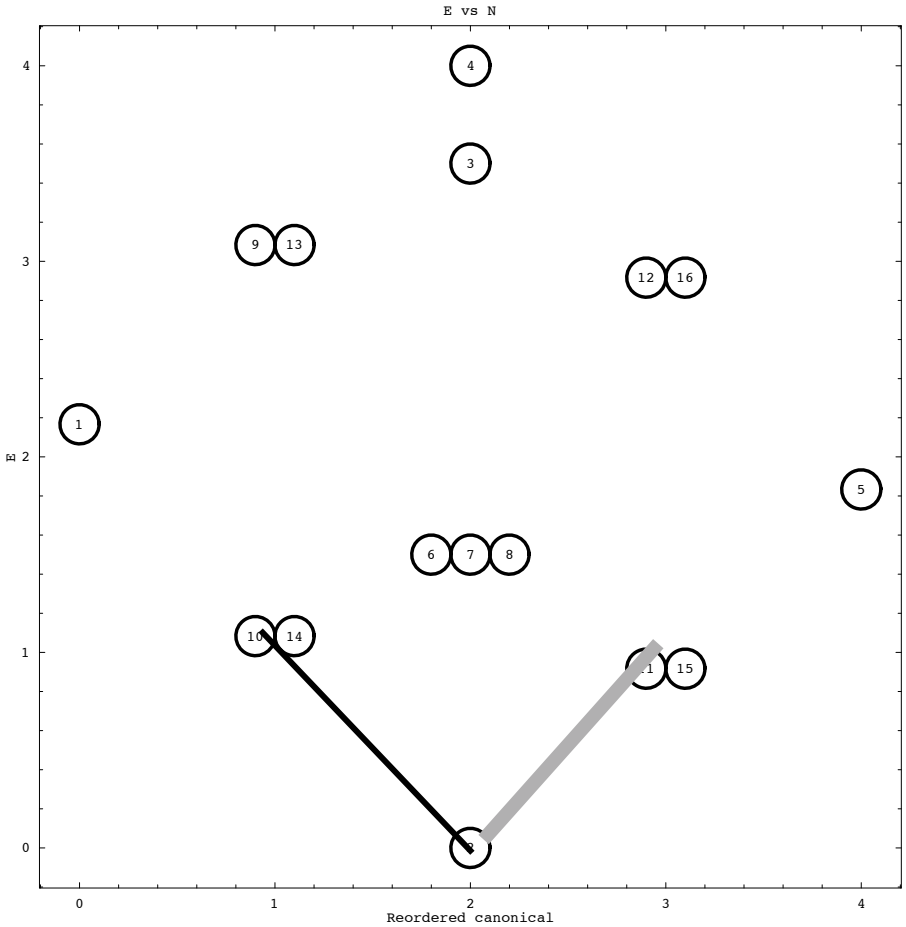
We permute these states



$\epsilon_d = -\frac{1}{2}U$ and $V = 2, U = 8$.

$$\epsilon_d\, n_d + U\, n_{d\uparrow} \cdot n_{d\downarrow} + V\, \Sigma_\sigma (c^\dagger_{0,\sigma} d_\sigma + CC)$$





$$n_{tot} + \frac{1}{12}(n_a - n_b) - \frac{1}{2} S_a \cdot S_b$$

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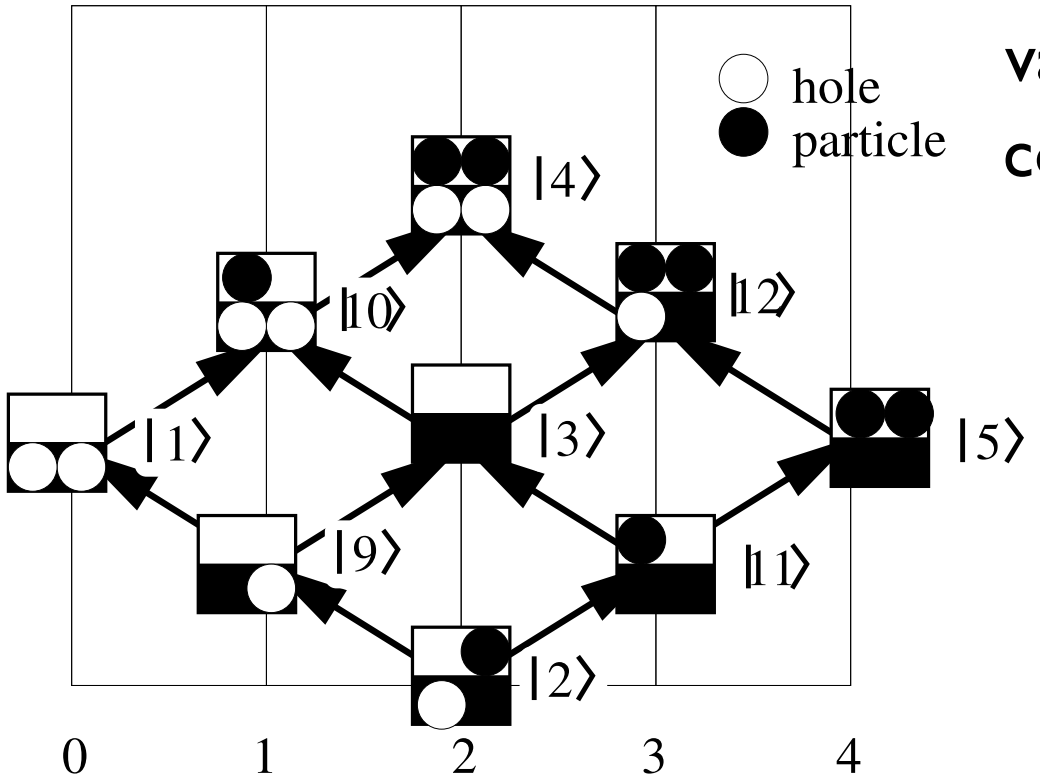
$$\epsilon_d \, n_d + U \, n_{d\uparrow} \cdot n_{d\downarrow} + V \, \Sigma_\sigma (c^\dagger_{0,\sigma} d_\sigma + CC)$$

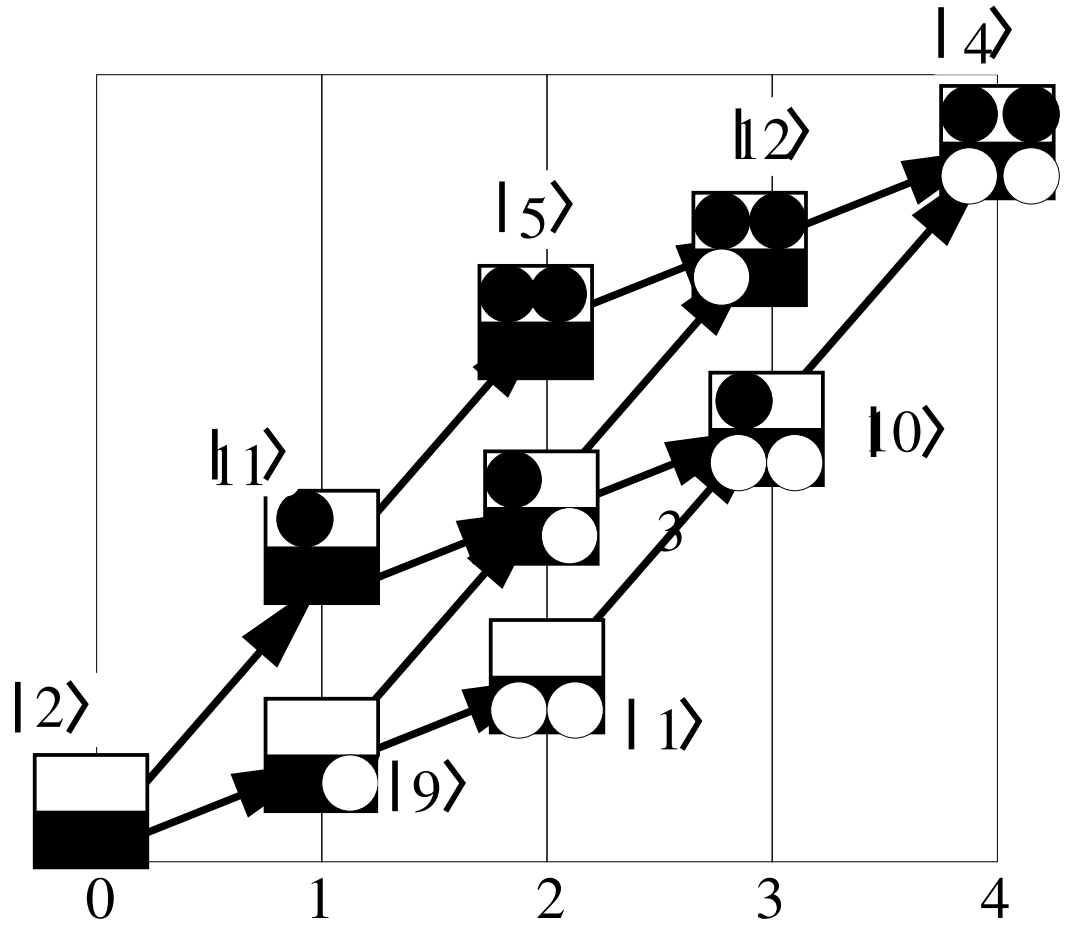
Pictogram of the interacting state



valence hole

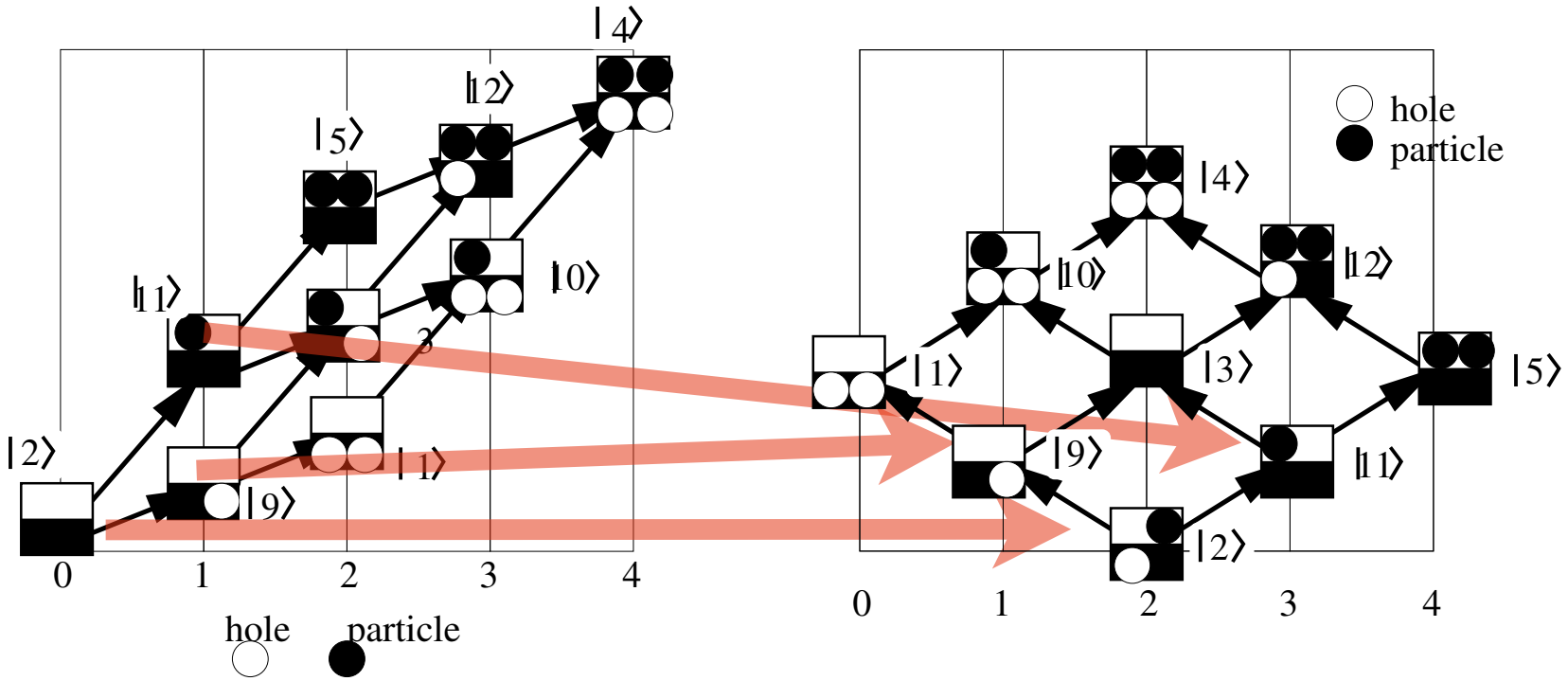
conduction particle

$$(n_e + \gamma n_h)VS(n_e + n_h)$$



quasihole ○ quasielectron ●

$$(n_e + \gamma n_h) V S (n_e + n_h)$$



A permutation is a canonical transformation ** and can be represented by:

$$U = P(\hat{c}_e, \hat{c}_h, \hat{c}_e^\dagger, \hat{c}_h^\dagger)$$

Invert this

$$c_c^\dagger = U^\dagger \hat{c}_e^\dagger U$$

$$c_f = U^\dagger \hat{c}_h^\dagger U$$

This transformation is then done **exactly** with computer algebra ....

This reordering generates a canonical transformation that by construction maps states properly

$$c^{\dagger}_{c,\uparrow} = \hat{c}_{h,\downarrow}\left(\tau_2 n_{e,\downarrow} + \frac{1}{2}\hat{c}^{\dagger}_{h,\uparrow}\hat{c}^{\dagger}_{e,\downarrow} - \tau_1 n_{e,\uparrow} - \frac{1}{\sqrt{2}} n_{h,\uparrow}\right)$$

$$+ \hat{c}^{\dagger}_{e,\uparrow}\left(\tau_1 n_{h,\downarrow} + \frac{-1}{2}\hat{c}_{h,\uparrow}\hat{c}_{e,\downarrow} + \frac{1}{\sqrt{2}} n_{e,\downarrow} - \tau_2 n_{h,\uparrow}\right)$$

$$+ \left(\frac{1}{\sqrt{2}}\hat{c}_{h,\downarrow} - \frac{1}{\sqrt{2}}\hat{c}^{\dagger}_{e,\uparrow}\right) + \cdots,$$

$$\tau_2 = (1 - 1/\sqrt{2}) \text{ and } \tau_1 = \tfrac{1}{2}(\sqrt{2} - 1).$$

This reordering generates a canonical transformation that by construction maps states properly

$$c^{\dagger}_{c,\uparrow} = \hat{c}_{h,\downarrow}\left(\tau_2 n_{e,\downarrow} + \frac{1}{2}\hat{c}^{\dagger}_{h,\uparrow}\hat{c}^{\dagger}_{e,\downarrow} - \tau_1 n_{e,\uparrow} - \frac{1}{\sqrt{2}} n_{h,\uparrow} \right)$$

$$+ \hat{c}^{\dagger}_{e,\uparrow}\left(\tau_1 n_{h,\downarrow} + \frac{-1}{2}\hat{c}_{h,\uparrow}\hat{c}_{e,\downarrow} + \frac{1}{\sqrt{2}} n_{e,\downarrow} - \tau_2 n_{h,\uparrow} \right)$$

$$+ \left(\frac{1}{\sqrt{2}}\hat{c}_{h,\downarrow} - \frac{1}{\sqrt{2}}\hat{c}^{\dagger}_{e,\uparrow} \right) + \cdots ,$$

"Bogoliubov"

$$\tau_2 = (1 - 1/\sqrt{2}) \text{ and } \tau_1 = \tfrac{1}{2}(\sqrt{2} - 1).$$

$$c^{\dagger}_{f,\uparrow} = \hat{c}^{\dagger}_{e,\uparrow}\left(\frac{1}{2}n_{h,\downarrow} + n_{e,\downarrow} + \frac{-1}{2}\hat{c}_{h,\uparrow}\hat{c}_{e,\downarrow} + \frac{1}{\sqrt{2}}\hat{c}^{\dagger}_{h,\uparrow}\hat{c}^{\dagger}_{e,\downarrow}\right)$$

$$+ \hat{c}_{h,\downarrow}\left(\frac{-1}{2}n_{e,\uparrow} + \frac{1}{2}\hat{c}^{\dagger}_{h,\uparrow}\hat{c}^{\dagger}_{e,\downarrow} - \frac{1}{\sqrt{2}}\hat{c}_{h,\uparrow}\hat{c}_{e,\downarrow} - n_{h,\uparrow}\right) + \cdots .$$

Note no Bogoliubov-like terms

We get an exact mapping to electrons and holes

$$n_{tot} = 2 + \hat{c}^{\dagger}_{e,\uparrow}\,\hat{c}_{e,\uparrow} + \hat{c}^{\dagger}_{e,\downarrow}\,\hat{c}_{e,\downarrow} - \hat{c}^{\dagger}_{h,\downarrow}\,\hat{c}_{h,\downarrow} - \hat{c}^{\dagger}_{h,\uparrow}\,\hat{c}_{h,\uparrow}$$

The local atomic Kondo interaction becomes

$$\begin{aligned} H_{KLM} = \; & 3Jn_e + \tfrac{1}{4}n_e(n_e-1)(-6J+U_f) + \\ & \tfrac{1}{8}n_e(n_e-1)n_h(6J-U_f) + \tfrac{1}{8}n_e n_h(-18J+U_f) + \\ & \tfrac{1}{8}n_e n_h(n_h-1)(6J-U_f) + 3Jn_h + \\ & \tfrac{1}{4}n_h(n_h-1)(-6J+U_f) + \tfrac{1}{8}(S_c\cdot S_f)(2J-U_f) \end{aligned}$$

For the record, the exact transformation can be written down and used but the details are not interesting

$$
\begin{aligned}
c^{\dagger}_{c,\uparrow} = \; & \hat{c}_{h,\downarrow}\,(\tau_1\, n_{h,\uparrow}\, n_{e,\uparrow} + \tau_2\, n_{e,\downarrow} + \tau_1\, n_{h,\uparrow}\, n_{e,\downarrow} + \tau_1\, n_{e,\uparrow}\, n_{e,\downarrow} + \tfrac{1}{2}\,\hat{c}^{\dagger}_{h,\uparrow}\,\hat{c}^{\dagger}_{e,\downarrow} - \tau_1\, n_{e,\uparrow} - \tfrac{1}{\sqrt{2}}\, n_{h,\uparrow}) \; + \\
& \hat{c}^{\dagger}_{e,\uparrow}\,(\tau_1\, n_{h,\downarrow} + \tfrac{-1}{2}\,\hat{c}_{h,\uparrow}\,\hat{c}_{e,\downarrow} + \tfrac{1}{\sqrt{2}}\, n_{e,\downarrow} - \tau_1\, n_{h,\downarrow}\, n_{e,\downarrow} - \tau_1\, n_{h,\uparrow}\, n_{e,\downarrow} - \tau_1\, n_{h,\uparrow}\, n_{h,\downarrow} - \tau_2\, n_{h,\uparrow}) \; + \\
& (\tfrac{1}{\sqrt{2}}\,\hat{c}_{h,\downarrow} - \tfrac{1}{\sqrt{2}}\,\hat{c}^{\dagger}_{e,\uparrow})
\end{aligned}
$$

$$
\begin{aligned}
c^{\dagger}_{f,\uparrow} = \; & \hat{c}^{\dagger}_{e,\uparrow}\,(\tfrac{1}{2}\, n_{h,\downarrow} + \tfrac{-1}{2}\, n_{h,\uparrow}\, n_{h,\downarrow} + n_{e,\downarrow} + \tfrac{-1}{2}\, n_{h,\uparrow}\, n_{e,\downarrow} + \tfrac{-1}{2}\, n_{h,\downarrow}\, n_{e,\downarrow} + \tfrac{-1}{2}\,\hat{c}_{h,\uparrow}\,\hat{c}_{e,\downarrow} + \tfrac{1}{\sqrt{2}}\,\hat{c}^{\dagger}_{h,\uparrow}\,\hat{c}^{\dagger}_{e,\downarrow}) \; + . \\
& \hat{c}_{h,\downarrow}\,(\tfrac{-1}{2}\, n_{e,\uparrow} + \tfrac{1}{2}\, n_{h,\uparrow}\, n_{e,\uparrow} + \tfrac{1}{2}\, n_{h,\uparrow}\, n_{e,\downarrow} + \tfrac{1}{2}\, n_{e,\uparrow}\, n_{e,\downarrow} + \tfrac{1}{2}\,\hat{c}^{\dagger}_{h,\uparrow}\,\hat{c}^{\dagger}_{e,\downarrow} - \tfrac{1}{\sqrt{2}}\,\hat{c}_{h,\uparrow}\,\hat{c}_{e,\downarrow} - n_{h,\uparrow})
\end{aligned}
$$

$\tau_2 = (1 - 1/\sqrt{2})$ $\qquad$ $\tau_1 = \frac{1}{2}(\sqrt{2} - 1)$

The original Kondo Lattice model

$$H_{KLM} = -t \sum_{rr'} (c^{\dagger}_{c,\sigma}(r) c_{c,\sigma}(r') + CC) \; + \; \sum_{r} (J \; S_c(r) \cdot S_f(r) + U_f (n_f(r) - 1)^2 \,)$$

becomes a **dilute** fermi gas which is then truncated to a free fermion model in electron and hole operators

$$\begin{aligned} H^{eff}_{KLM} = \; & J(n_e(r) + n_h(r)) & + \\ & \Sigma_s \, (-1)^s t((\hat{c}^{\dagger}_{e,s}(r) \, \hat{c}^{\dagger}_{h,-s}(r') - \hat{c}_{e,s}(r') \, \hat{c}_{h,-s}(r) + CC \,)) & + \\ & \Sigma_s \, (t(\hat{c}^{\dagger}_{e,s}(r) \, \hat{c}_{e,s}(r') - \hat{c}^{\dagger}_{h,s}(r) \, \hat{c}_{h,s}(r')) + CC \,) \end{aligned}$$

(Note the the Hamiltonian is approximate but the transformation is exact. This is important when computing expectation values of functions of bare electron operators!)

Ground state energies accurate to $(t/J)^4$ *

$$E_k = \frac{3J}{4}\Delta_k \pm te_k \pm \mu \text{ where } \Delta_k = \sqrt{1+(\frac{4te_k}{3J})^2}.$$

$$\alpha = \frac{1}{2}\iiint_{T^d}(1-\Delta_k^{-1})\ (\frac{d\theta}{2\pi})^d$$

$$\beta = \iiint_{T^d} e_k^2/\Delta_k\ (\frac{d\theta}{2\pi})^d \approx \frac{d}{2} - \frac{d}{3}\lambda^2 + O(t^4)$$

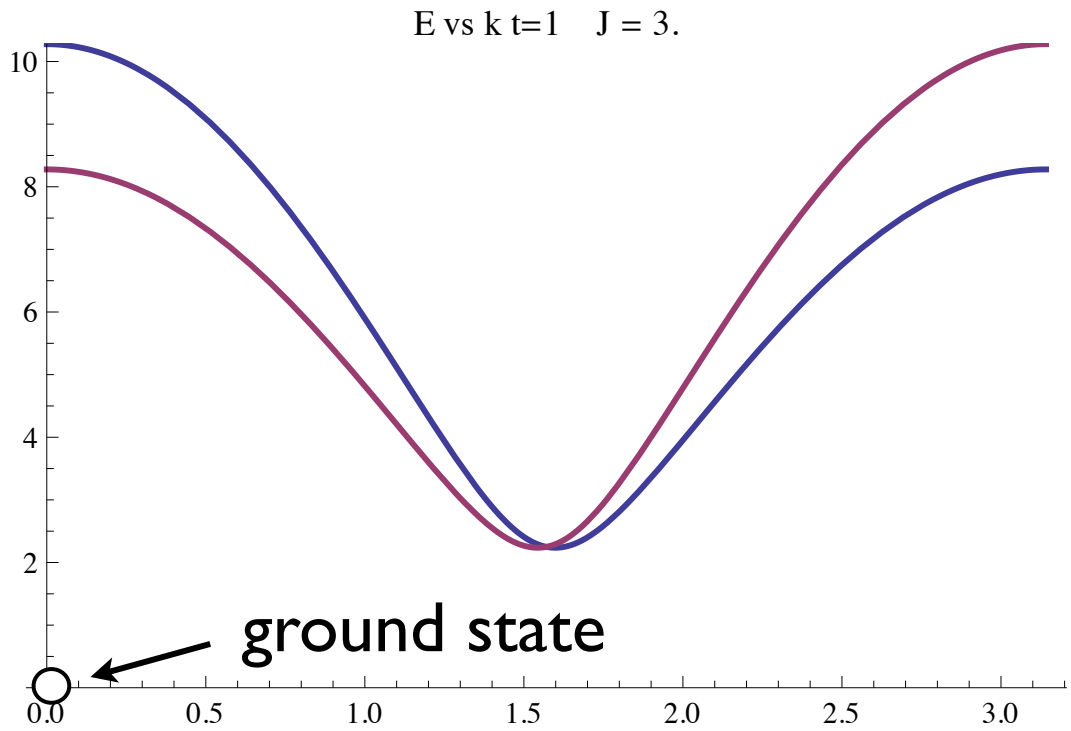
$$\langle\, H_{KLM}\,\rangle_{free} = \frac{-3}{4} + 3\,\alpha + \frac{-15}{4}\,\alpha^2 + \frac{3}{2}\,\alpha^3 + \frac{-8}{3}\,\beta\,\lambda^2 \ + \quad .$$
$$\alpha^3\,\beta\,\lambda^2\,(72 + -48\,\sqrt{2}) + \alpha\,\beta^3\,d^{-2}\,\lambda^4\,(\frac{64}{3} + \frac{-128}{9}\,\sqrt{2}) \ +$$
$$\alpha\,\beta\,\lambda^2\,(16 + -8\,\sqrt{2}) + \beta^5\,d^{-4}\,\lambda^6\,(\frac{-64}{27} + \frac{128}{81}\,\sqrt{2}) \ +$$
$$\beta^3\,d^{-2}\,\lambda^4\,(\frac{-64}{9} + \frac{32}{9}\,\sqrt{2}) + \alpha^2\,\beta^3\,d^{-2}\,\lambda^4\,(\frac{-64}{3} + \frac{128}{9}\,\sqrt{2}) \ +$$
$$\alpha^4\,\beta\,\lambda^2\,(-36 + 24\,\sqrt{2}) + \alpha^2\,\beta\,\lambda^2\,(-52 + 32\,\sqrt{2})$$

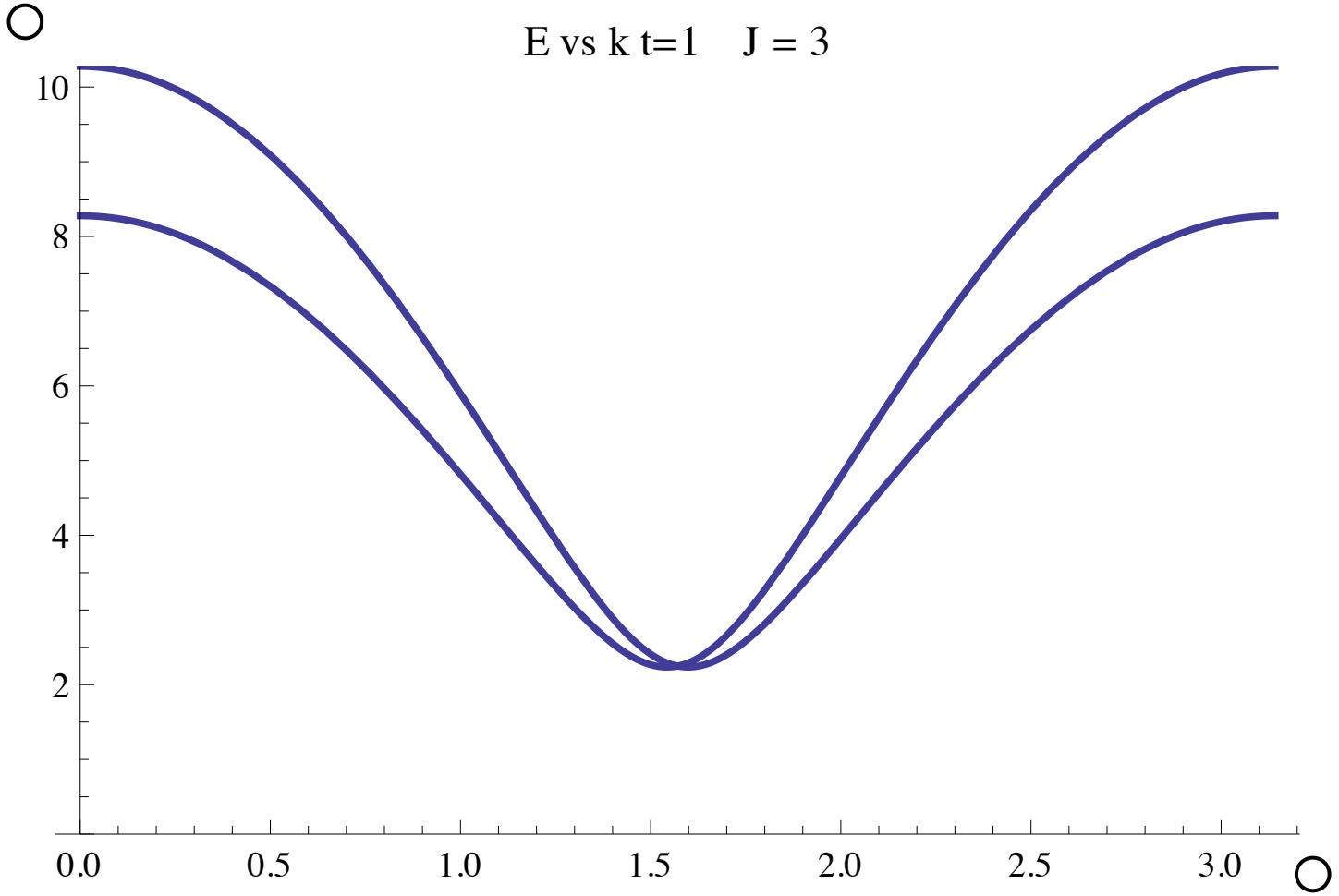
** Zheng and Oitmaa, 2003*

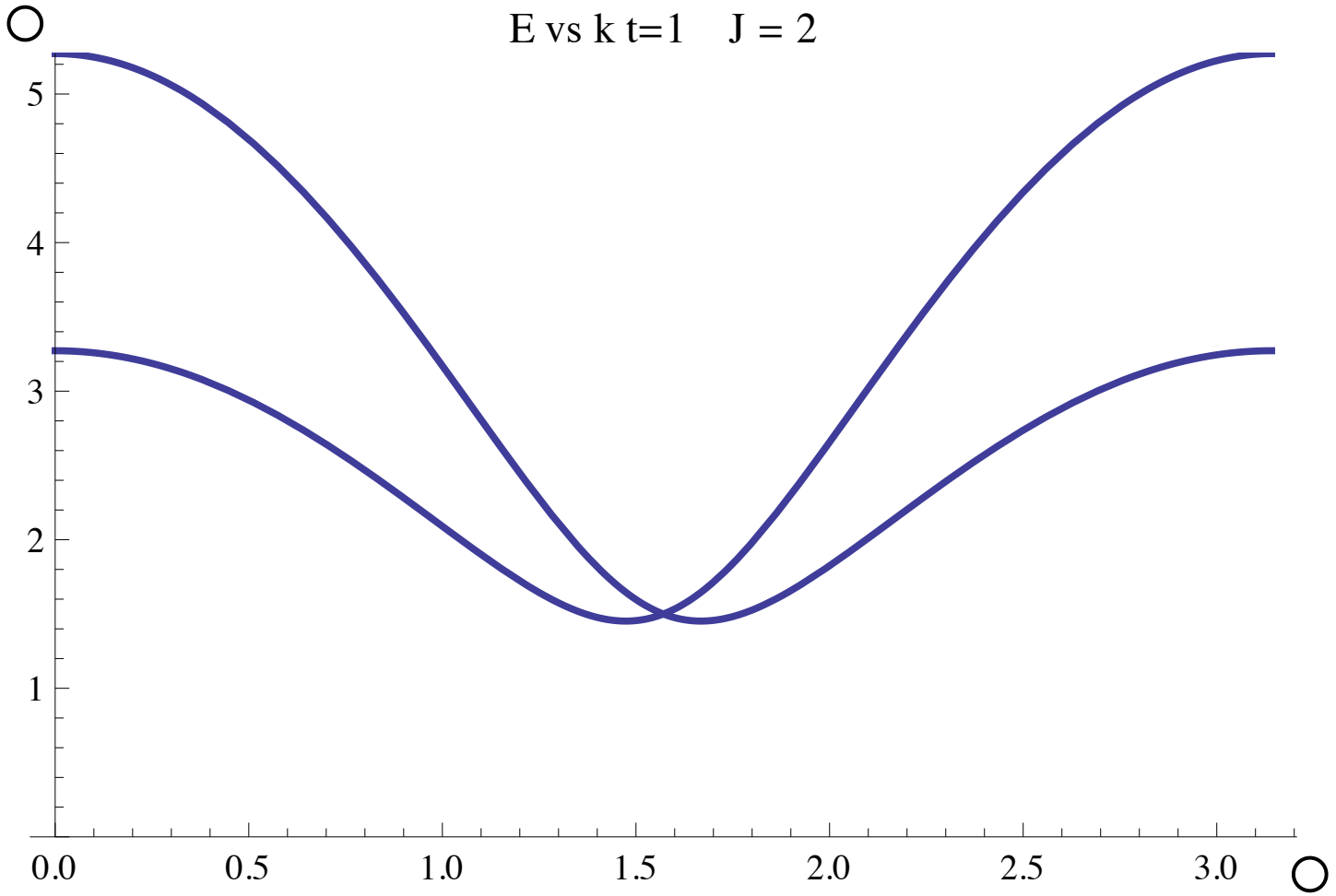
Spectrum and spectral weights can be computed with the exact canonical transformation but with the approximate Hamiltonian.

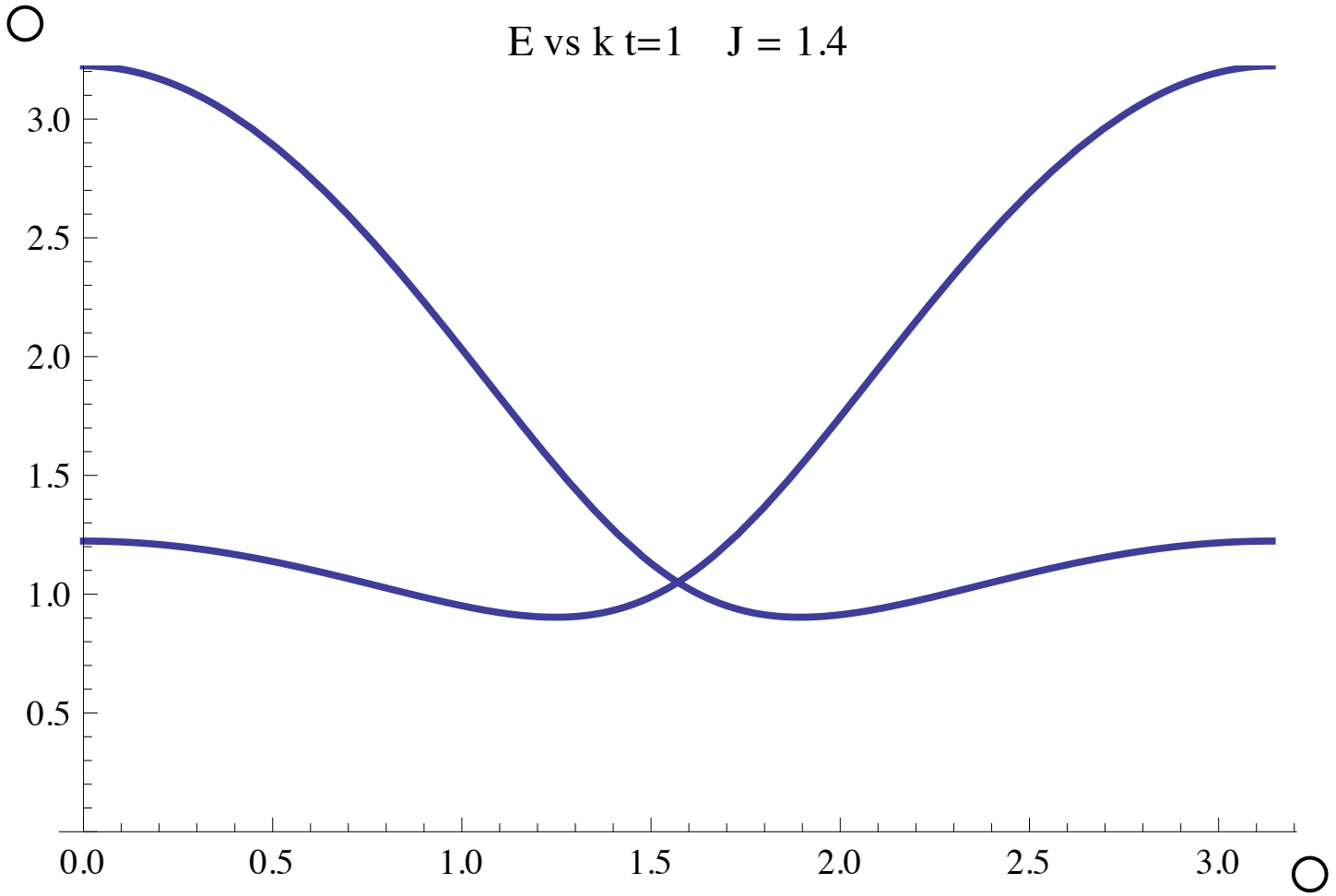
$$\Delta_k = \sqrt{1 + (\frac{4te_k}{3J})^2}.$$

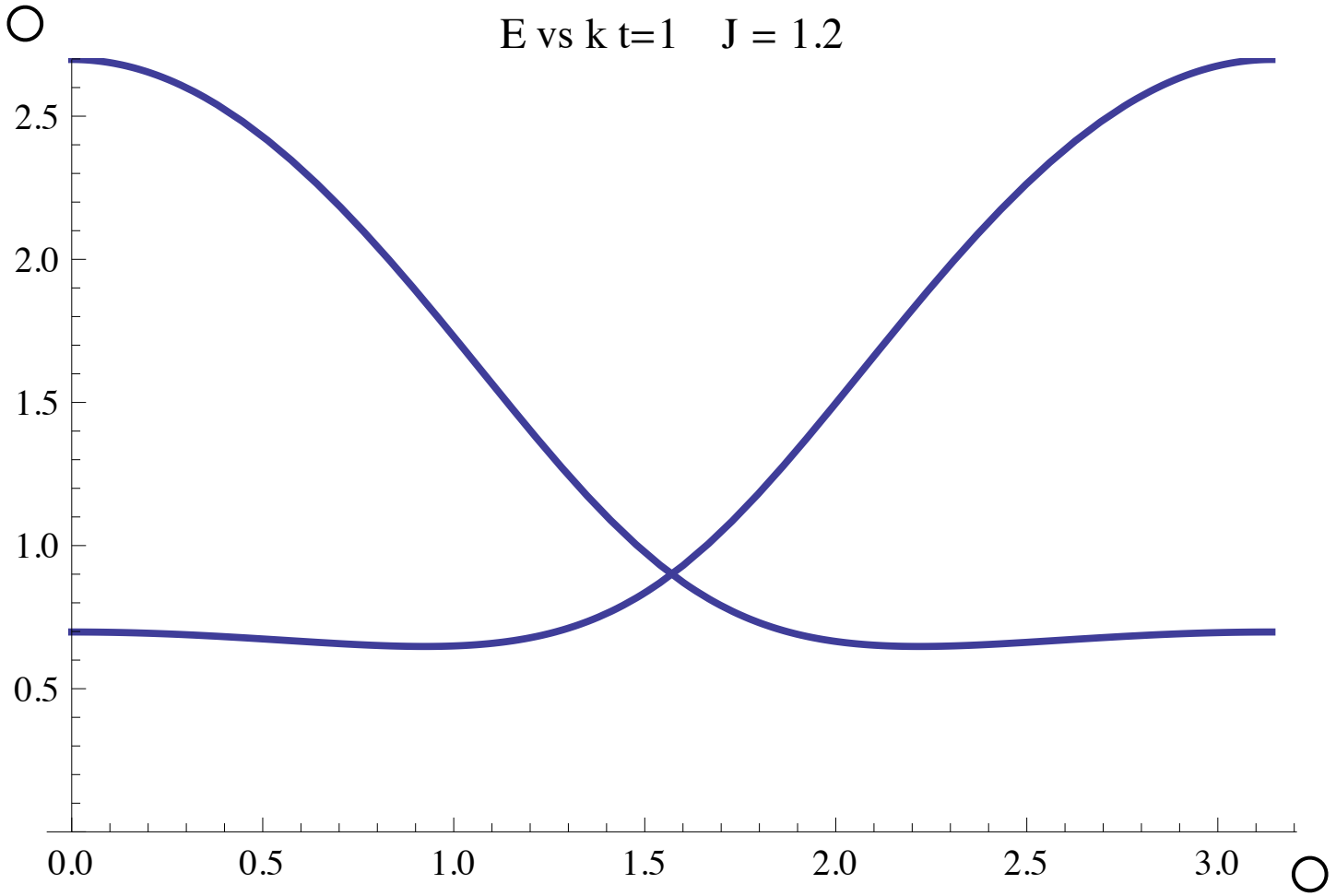
$$E_k = \frac{3J}{4}\Delta_k \pm te_k \pm \mu$$

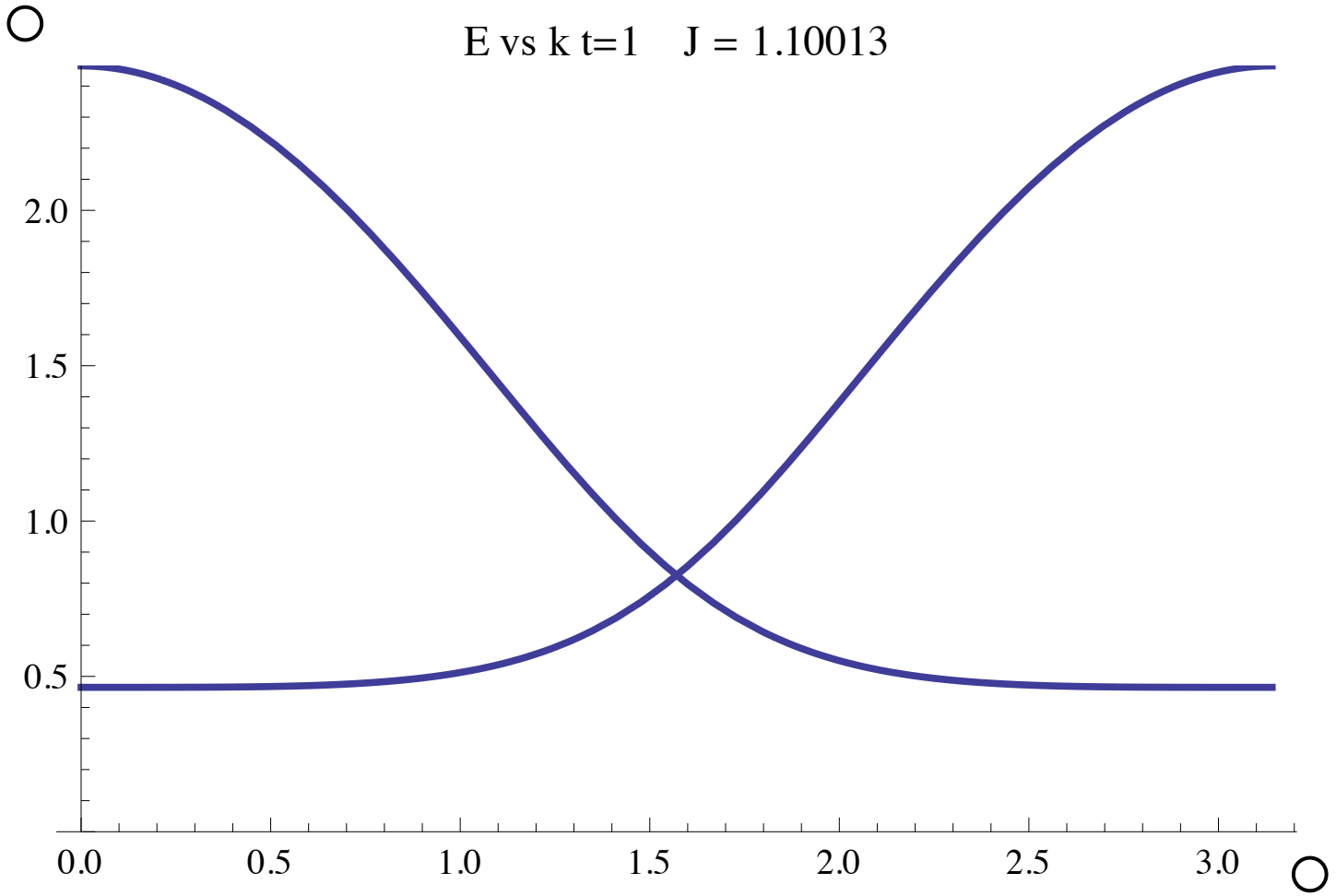


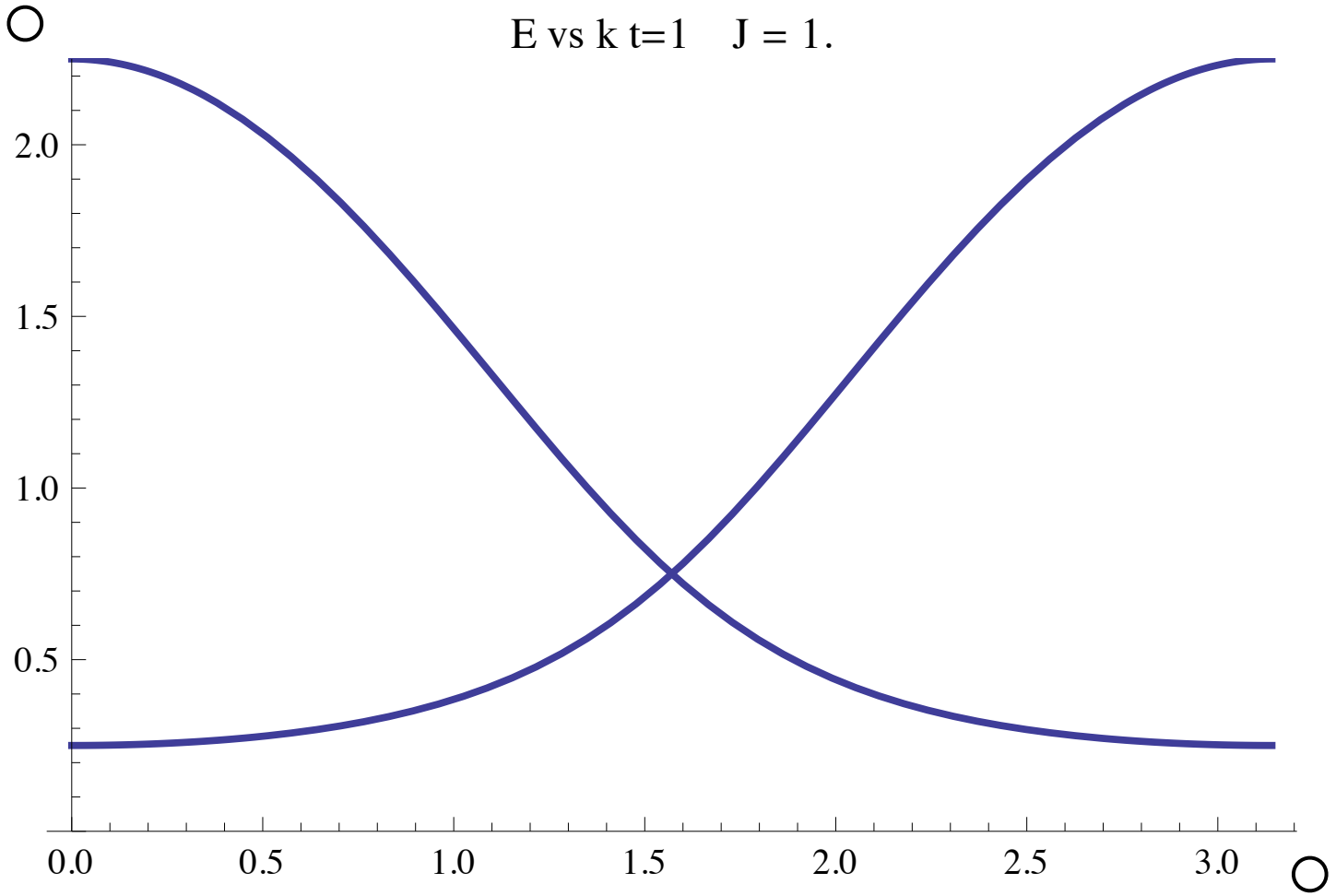

E vs k t=1 J = 3
10
8
6
4
2
0.0
0.5
1.0
1.5
2.0
2.5
3.0

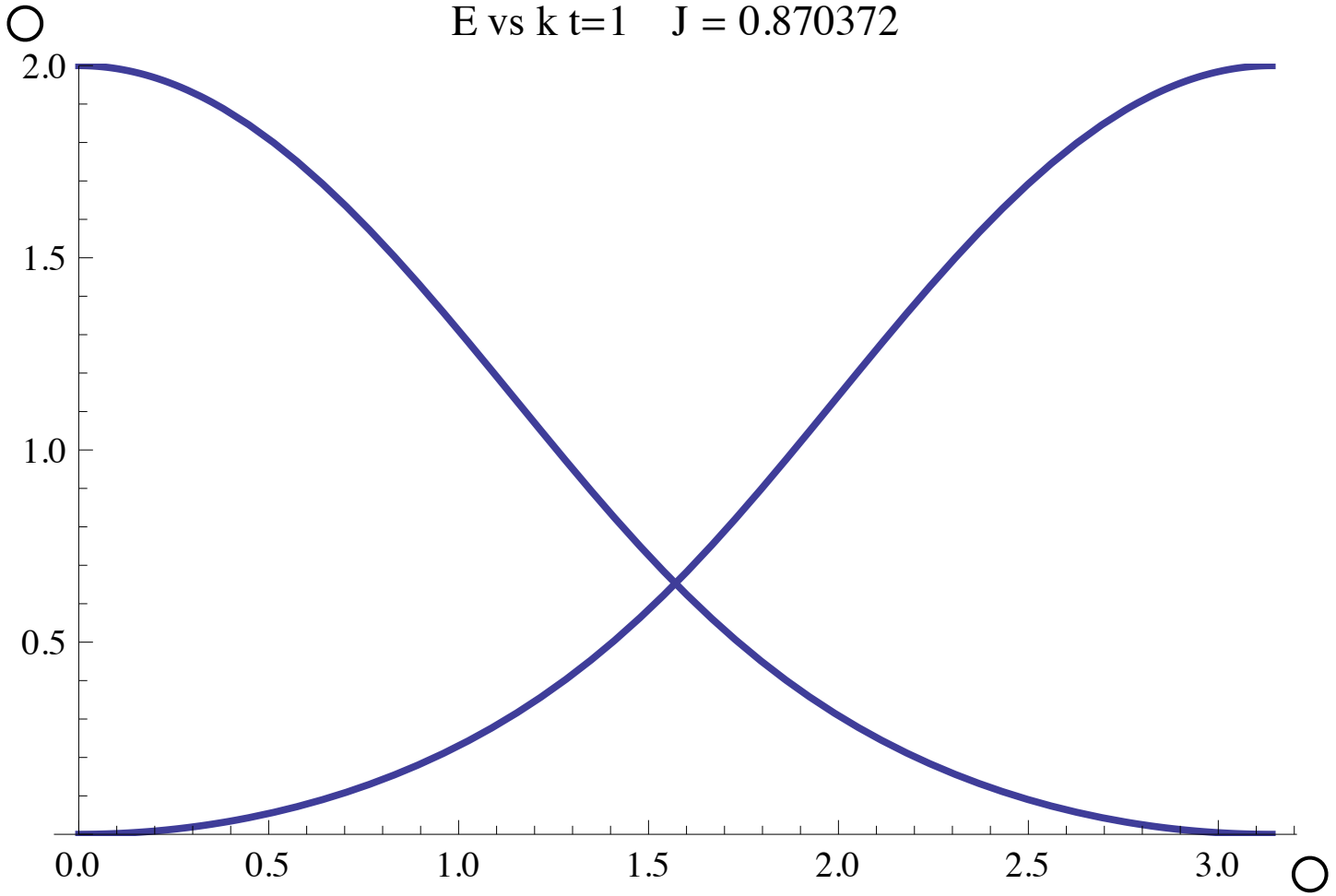

E vs k t=1 J = 2
5
4
3
2
1
0.0
0.5
1.0
1.5
2.0
2.5
3.0

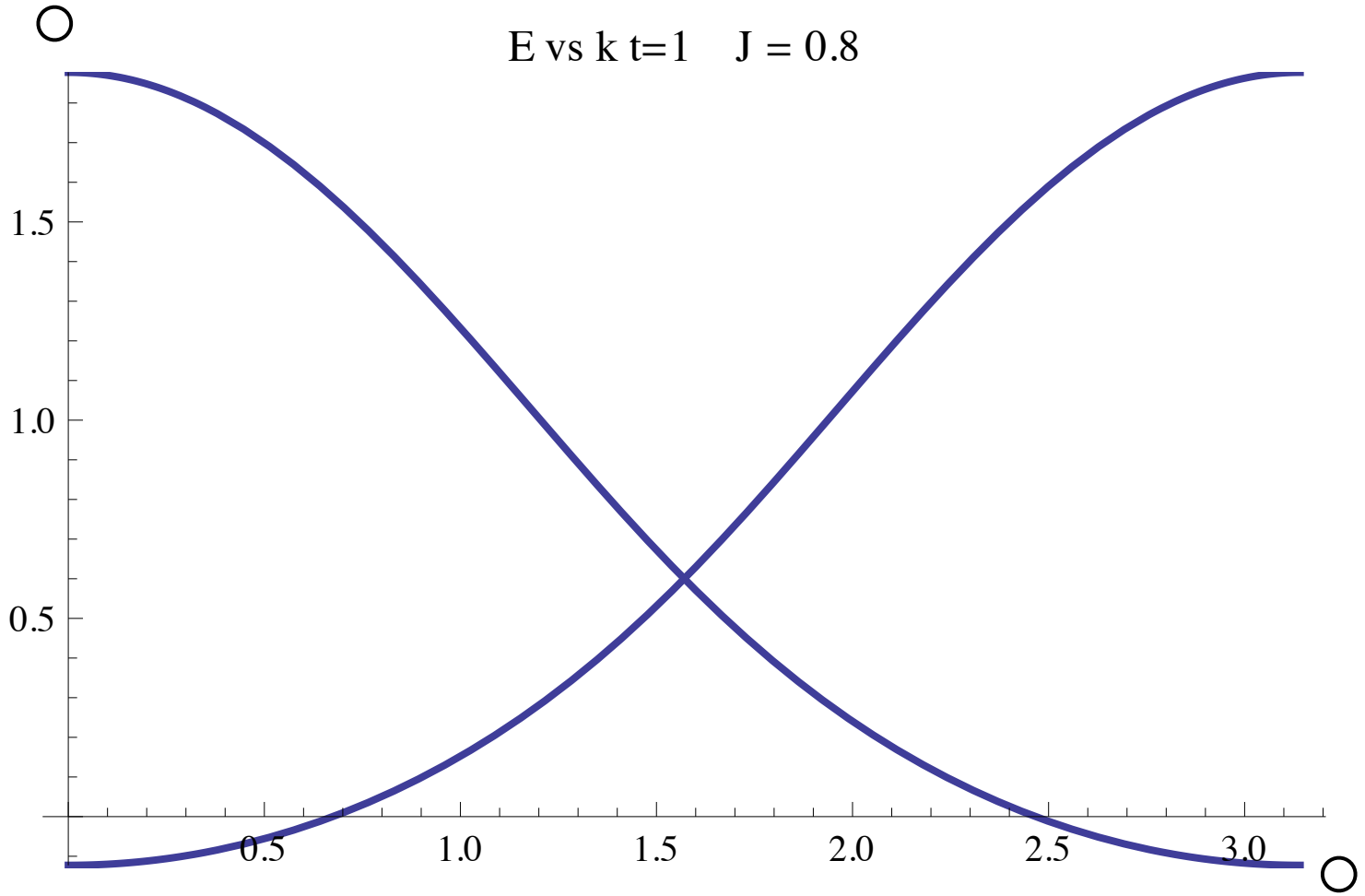

E vs k t=1 J = 1.4
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0

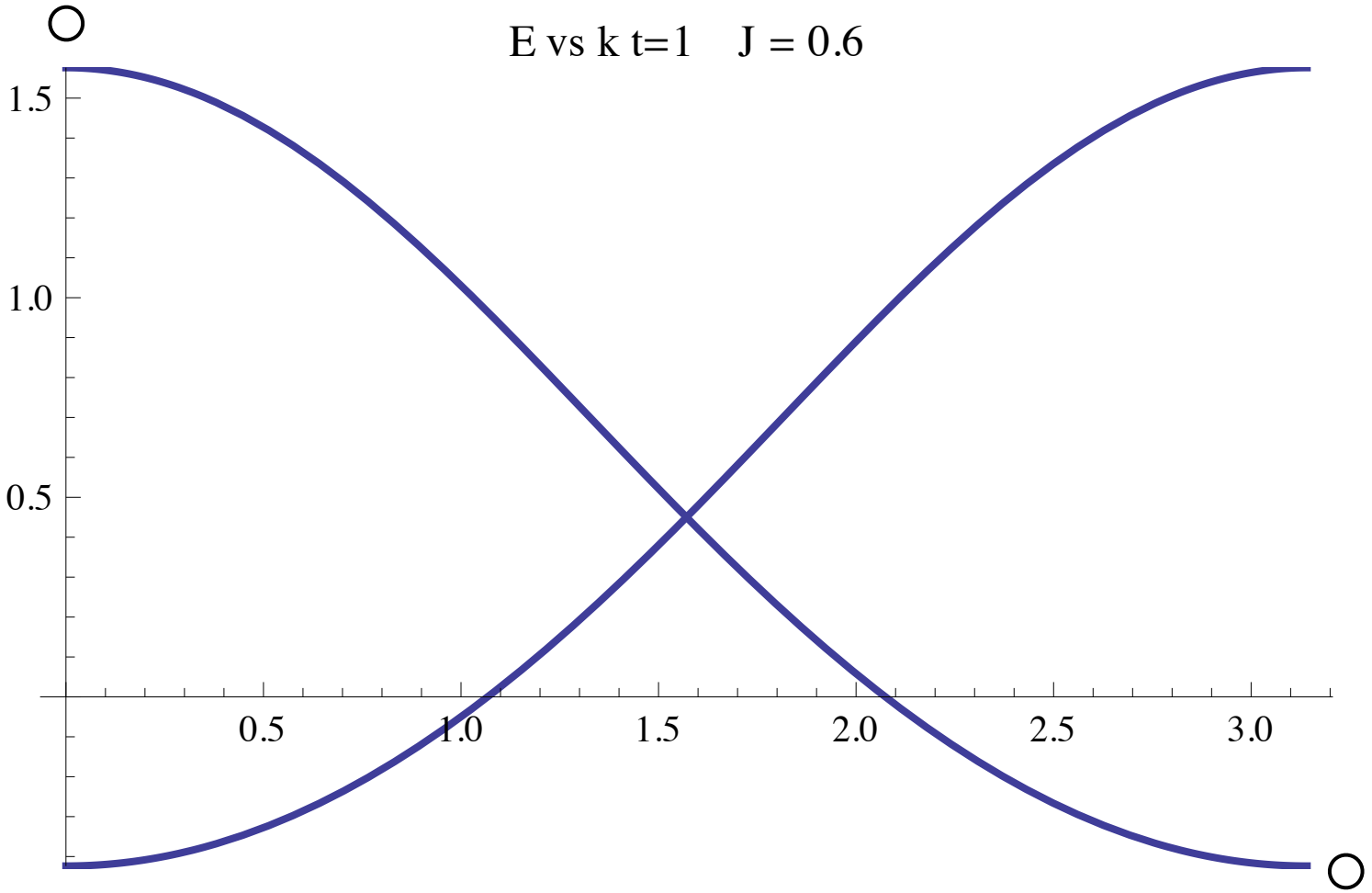

E vs k t=1 J = 1.2
2.5
2.0
1.5
1.0
0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0

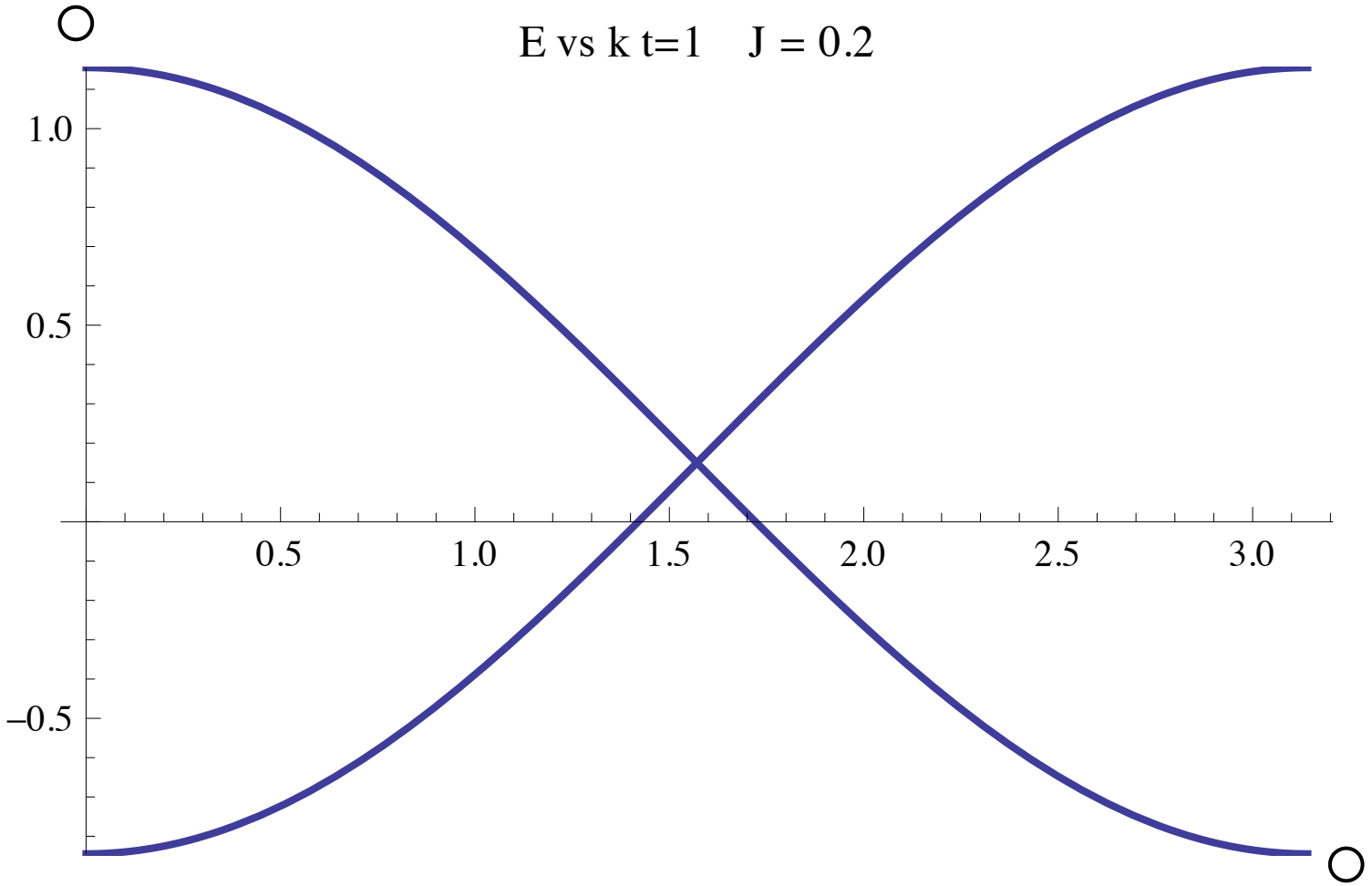

E vs k t=1 J = 1.10013
2.0
1.5
1.0
0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0

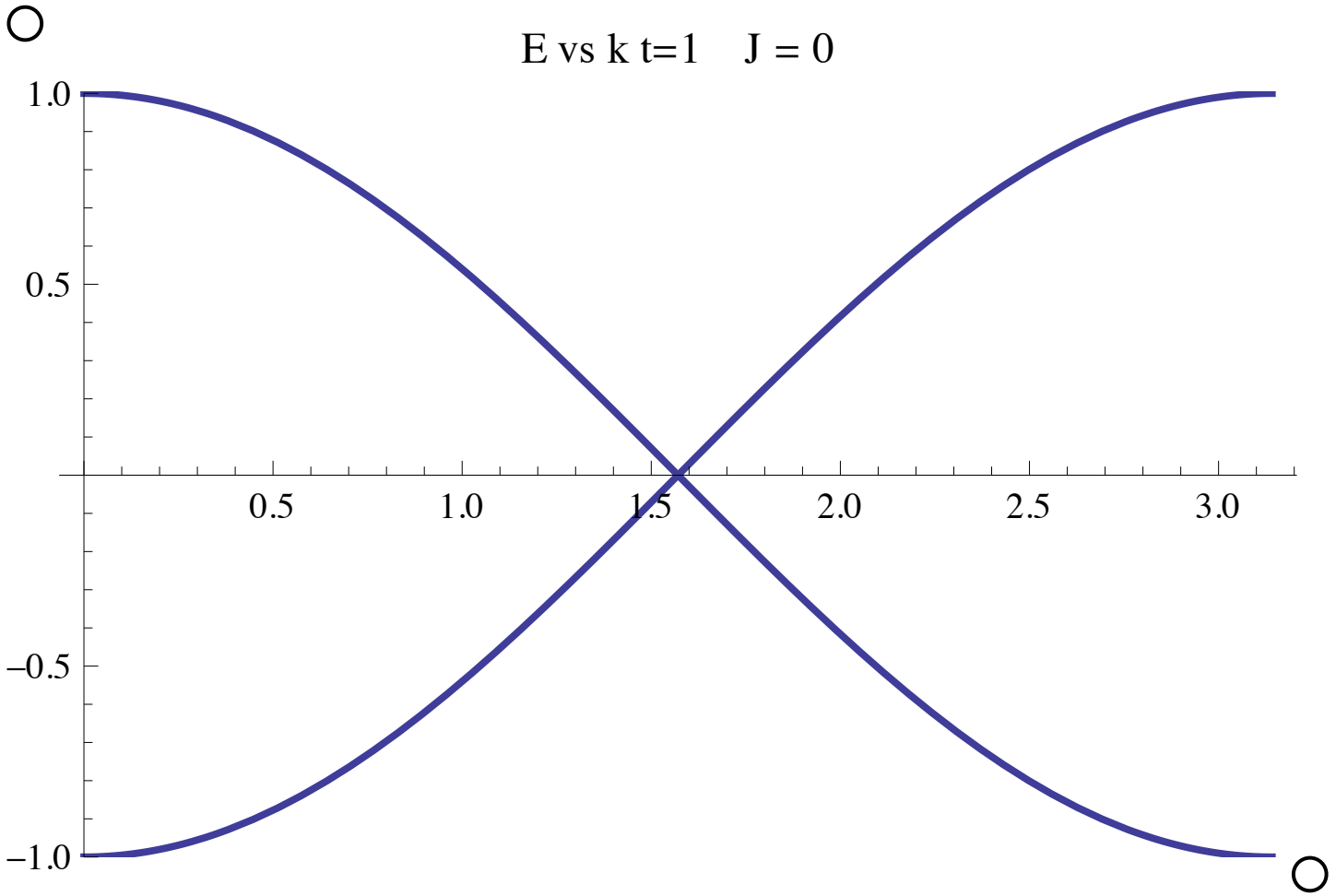

E vs k t=1 J = 1.
2.0
1.5
1.0
0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0


E vs k t=1 J = 0.870372
2.0
1.5
1.0
0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0

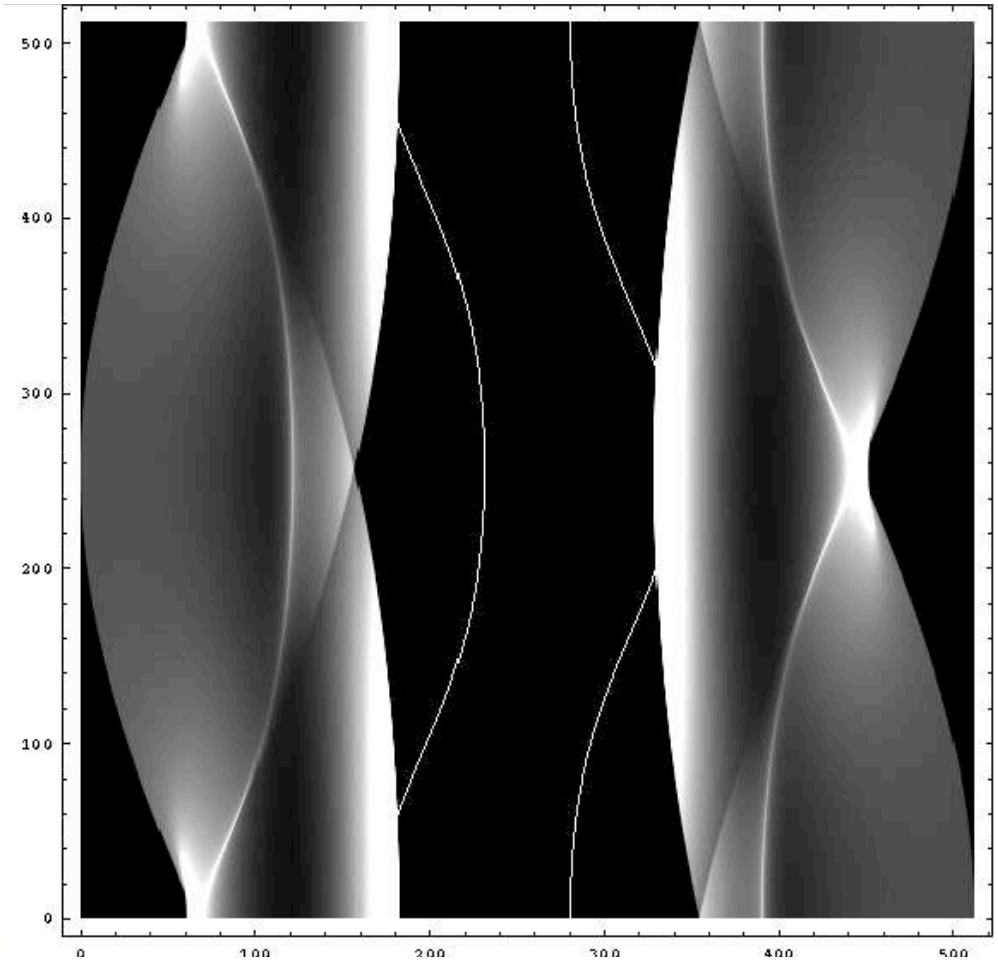

E vs k t=1 J = 0.8
1.5
1.0
0.5
0.5
1.0
1.5
2.0
2.5
3.0


E vs k t=1 J = 0.6
1.5
1.0
0.5
0.5
1.0
1.5
2.0
2.5
3.0


E vs k t=1 J = 0.2
1.0
0.5
–0.5
0.5
1.0
1.5
2.0
2.5
3.0


E vs k t=1 J = 0
1.0
0.5
–0.5
–1.0
0.5
1.0
1.5
2.0
2.5
3.0

c-electron spectral weight



Note delta function component together with a continuous scattering part.

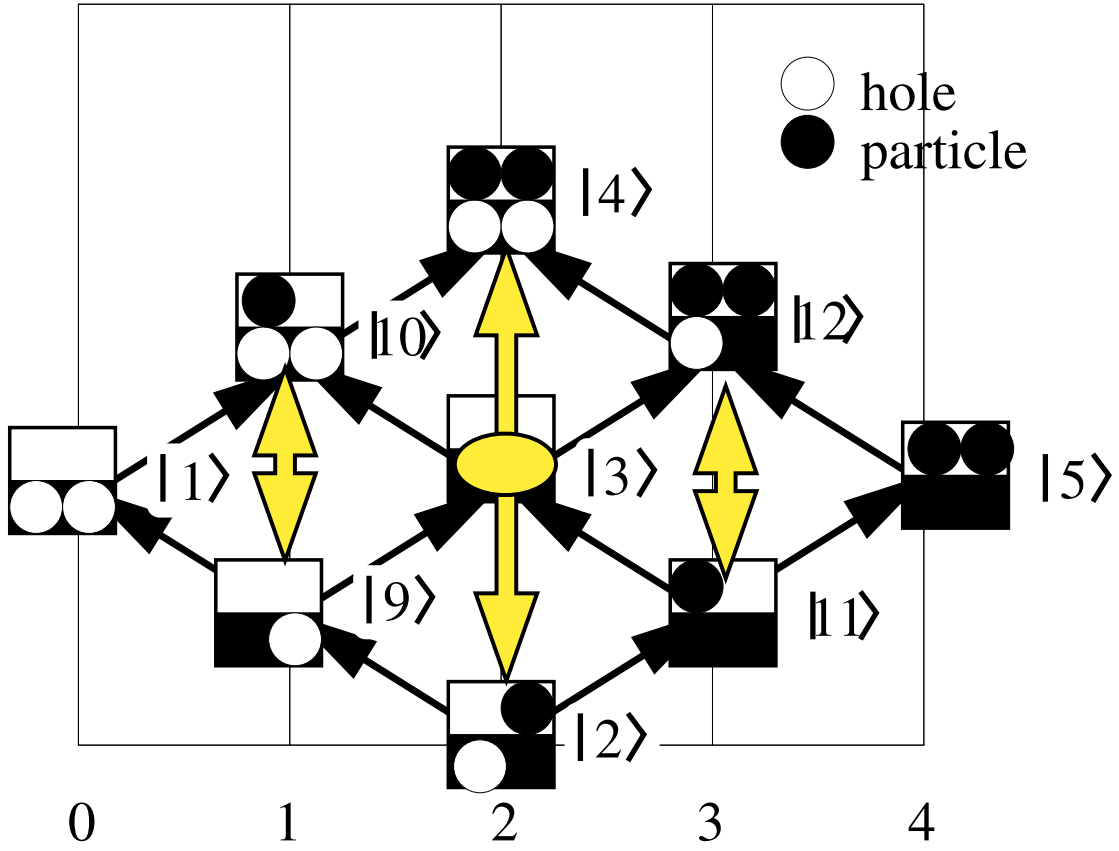
Generalizations:

Transformations can be generalized from fixed permutation to

$$SU(2) \otimes SU(3) \otimes SU(2)$$

that can continuously rotate from the identity transfromation (weak coupling) to strong coupling permutation

Transformations can be generalized to $SU(2) \otimes SU(3) \otimes SU(2)$



$SU(2) \otimes SU(3) \otimes SU(2)$

An approximate free quasiparticle model can be constructed which can describe a type of metal-insulator transition for which spectrum and bare electron spectral weights can be computed exactly

Conclusion for the Kondo Lattice model

Exact "nonlinear" canonical transformations can be constructed that maps the Kondo Lattice Model to a dilute gas of fermions in the strong coupling limit and should be applicable to other even valence insulators.

The method reproduces accurate results $(t/J)^4$ in this limit while preserving the spectral weight sum rules, whose violation have plagued previous investigations with using approximate transformations.

The bare electrons are naturally described as composite quasiparticle operators.

Exactly solvable impurity models that may retain some strong coupling physics can be analyzed exactly

Can we apply these ideas to Hubbard model?

Previous method does not work for odd valence insulator.

$$H = -t \sum_{\langle rr' \rangle} (c^{\dagger}_{s,r} c_{s,r'} + CC) + U \sum_r \tfrac{1}{2} (n_r - 1)^2$$

The ground state consists of one electron per site. Consider the Neel ground state. Can we make a unitary transformation that maps one of the two ***one-particle*** states to the "Fermi" vacuum consisting of zero particles.

Guided by previous studies of 'nonlinear' canonical transformation, it turns out that the following ***noncanonical*** transformation to accomplishes this without restricting the Hilbert space:

$$
\begin{aligned}
\hat{c}_r &= c^{\dagger}_{\downarrow,r}(1-n_{\uparrow,r}) + -1^r c_{\downarrow,r} n_{\uparrow,r} \\
q^{+}_r &= (c^{\dagger}_{\downarrow,r} - (-1)^r c_{\downarrow,r}\ )\ c_{\uparrow,r} \\
q^{-}_r &= (q^{+}_r)^{\dagger} \\
q^{z}_r &= \tfrac{1}{2} - n_{\uparrow,r}
\end{aligned}
$$

This exactly converts the algebra generated by two Fermionic spin degrees of freedom exactly to a 'quasicharge' Fermionic 'CP and a 'quasispin' Bosonic $SU(2)$

$$\{\hat{c}_r, \hat{c}^\dagger_{r'}\} = \delta_{r,r'}$$

$$\{\hat{c}^\dagger_r, \hat{c}^\dagger_{r'}\} = 0$$

$$\left[\, \hat{c}^\dagger_r, q^i_{r'} \,\right] = 0 \ ;$$

$$\left[\, q^i_r, q^j_{r'} \right] = i\delta_{rr'} \sum_k \epsilon_{ijk} q^k_r$$

The hopping splits into three pieces

$$H = t\left(T_0 + T_1 + T_{-1}\right) + U h_U$$

$$\begin{aligned}
T_0 &= \frac{1}{2}\sum_{\langle r,r'\rangle}(1+4q_r q_{r'})(\hat{c}_r^\dagger \hat{c}_{r'} + CC) \\
T_1 &= \frac{1}{2}\sum_{\langle r,r'\rangle} -1^r\,(1-4q_r q_{r'})(\hat{c}_r^\dagger \hat{c}_{r'}^\dagger) \\
T_{-1} &= \frac{1}{2}\sum_{\langle r,r'\rangle} -1^r\,(1-4q_r q_{r'})(\hat{c}_{r'} \hat{c}_r) \\
h_U &= \tfrac{1}{2}\sum_r \hat{c}_r^\dagger \hat{c}_r
\end{aligned}$$

The Hubbard interaction has become a chemical potential for the quasicharge operators.

Conclusions

- These arguments suggest that the free electrons must be nonperturbatively rewritten as composite operators in a strongly interacting system.
- Nonlinear canonical transformations are natural tools to study doped even values Mott insulators at least in the strong coupling limit.
- A natural generalization of this leads to exact nonunitary transformations that give charge-like fermionic and bosonic spin-like degrees of freedom.