A New Iterative Equation for Effective Interaction

Ryoji Okamoto
(Kyushu Institute of Technology, Japan)
Kenji Suzuki
(Kyushu Institute of Technology, Japan)
Hiroo Kumagai
(Fukuoka Institute of Technology, Japan)
Shinichiro Fujii
(CNS, University of Tokyo, Japan)

Plan of Talk

1. Introduction
2. Basic formulation
3. A schematic model analysis
4. Summary

10th Spring Seminar on Nuclear Structure @ Vietri sul Male, May 21-25, 2010

1.Introduction

In nuclear, atomic, chemical physics it is usually to recast the full many-body problem in the form of an **effective interaction** acting within a chosen model space for which the eigen values can be obtained exactly.

For a given set of non-folded diagrams, the folded diagram series can be summed by using either the **Krenciglowa-Kuo (KK)** technique[KK74] or the **Lee-Suzuki (LS) method** [LS80, SL80].

The KK approach, when convergent, yields the eigen values for those states which have the largest overlap with the chosen model space.[KK74]

The LS method reproduces those eigen values which lie closest to the chosen unperturbed energy.[SL80]

Andreozzi obtained another iterative techniques for effective interactions in the framework of non-orthogonal transformations.[Andr96]

It would be desirable to have a kind of **hybrid method of KK technique and LS method** which have some great merits in different aspects.
In this talk we propose a new method which could have essential merits of these two methods, and illustrate it in **a simple model analysis**.

2. Basic formulation

Hamiltonian and Schroedinger equation (true eigen value equations)

$$H = H_0 + V,$$

$$H|\psi_k\rangle = E_k|\psi_k\rangle, \quad \langle\psi_k|\psi_{k'}\rangle = \delta_{kk'}\ (k = 1, 2, \cdots, n)$$

Partition of the entire Hilbert space

$$P + Q = 1,\ P^2 = P,\ Q^2 = Q,\ PQ = QP = 0.$$

Basic assumption for the Hamiltonian

$$H_0 = PH_0P + QH_0Q$$

$$= E_0P + QH_0Q \quad \text{(degenerate model space)}$$

Model space eigen value equations

$$|\phi_k\rangle \equiv P|\psi_k\rangle, \rightarrow P = \sum_{k=1}^{d} |\phi_k\rangle\langle\tilde{\phi}_k|$$

$$\rightarrow \langle\phi_k|\phi_{k'}\rangle \neq \delta_{kk'}, \langle\tilde{\phi}_k|\phi_{k'}\rangle = \delta_{kk'}, |\tilde{\phi}_k\rangle; \text{bi-orthogonal states}$$

$$\rightarrow (E_0P + R)|\phi_k\rangle = E_k|\phi_k\rangle, \quad R = PRP$$

$$(k = 1, 2, \cdots, d < n), R: \text{non-Hermite effective interaction}$$

Definition of Q-box and its energy-derivative

$$\hat{Q}(E_k) \equiv PVP + PVQ\frac{1}{E_k - QHQ}QVP, \hat{Q}(E_k) = P\hat{Q}(E_k)P$$

$$\rightarrow \hat{Q}_m(E_k) \equiv \frac{1}{m!}\frac{\mathrm{d}^m \hat{Q}(E_k)}{\mathrm{d}E_k^m}, \hat{Q}_1(E_k) = -PVQ\frac{1}{(E_k - QHQ)^2}QVP$$

Krenciglowa-Kuo (KK) solution for effective interaction

$$R = \sum_{k=1}^{d} \hat{Q}(E_k)\left|\phi_k\right\rangle\left\langle\tilde{\phi}_k\right|$$

$$= \sum_{k=1}^{d} (E_k - E_0)\left|\phi_k\right\rangle\left\langle\tilde{\phi}_k\right|,$$

KK solution yields empirically to the largest P-state overlap state if it converges, but its convergence condition is not so clear.

The divergence of the perturbation expansion due to he presence of the intruder state

Lee-Suzuki method (vertex renormalization procedure) [SL80]

$$|\psi_k\rangle = (P+Q)|\psi_k\rangle = |\phi_k\rangle + \omega|\phi_k\rangle; \quad \omega = \sum_{k=1}^{d} Q|\psi_k\rangle\langle\tilde{\phi}_k|P, \omega^2 = 0, \cdots$$

$Qe^{-\omega}He^{\omega}P = 0$ Non-linear operator(matrix) equation [Andr96]

$\rightarrow QVP + QHQ\omega - \omega PHP - \omega PVQ = 0$: decoupling equation

$$\left[E_0 - (QHQ - \omega_{n-1}PVQ)\right]\omega_n = QVP - \omega_{n-1}PVP$$

$$\rightarrow R_1 = \hat{Q}, R_2 = \frac{1}{1-\hat{Q}_1}\hat{Q}, R_3 = \frac{1}{1-\hat{Q}_1 - \hat{Q}_2\left[1/(1-\hat{Q}_1)\right]\hat{Q}}\hat{Q}, \cdots$$

It converges to the eigen values nearest to the unperturbed starting energy.

A new iteration solution [*extended KK method, EKK*]

Based on Newton-Raphson (NR) method for a non-linear equation

Usual NR method: $f(x) = 0$ Modification; $F(x) \equiv x - f(x); x = F(x),$

$$\rightarrow x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$ Iteration eq.

$$\rightarrow x_{n+1} = \frac{F(x_n) - x_n F'(x_n)}{1 - F'(x_n)}$$ Iteration eq.

$x \Leftrightarrow (E - E_0), F(x) \Leftrightarrow \hat{Q}(E)$

$$\hat{Z}(E) \equiv \frac{1}{1-\hat{Q}_1(E)}\left[\hat{Q}(E) - (E-E_0)\cdot\hat{Q}_1(E)\right]; \text{'Z-box'}$$

$$R = \sum_{k=1}^{d} \hat{Z}(E_k)|\phi_k\rangle\langle\tilde{\phi}_k|$$

From KK solution for eff. Int.

$$(E_k - E_0)\left|\phi_k\right\rangle = R\left|\phi_k\right\rangle$$
$$= \hat{Q}(E_k)\left|\phi_k\right\rangle$$

Then we can prove the new equation (EKK) is a solution of the P-space effective interaction

$$\sum_{k=1}^{d} \frac{1}{1-\hat{Q}_1(E_k)}\left[\hat{Q}(E_k) - \hat{Q}_1(E_k)\cdot(E_k - E_0)\right]\left|\phi_k\right\rangle\left\langle\tilde{\phi}_k\right|$$
$$= \sum_{k=1}^{d} \frac{1}{1-\hat{Q}_1(E_k)}\left[R - \hat{Q}_1(E_k)\cdot R\right]\left|\phi_k\right\rangle\left\langle\tilde{\phi}_k\right|$$
$$= \sum_{k=1}^{d} \frac{1}{1-\hat{Q}_1(E_k)}\left[1 - \hat{Q}_1(E_k)\right]R\left|\phi_k\right\rangle\left\langle\tilde{\phi}_k\right|$$
$$= \sum_{k=1}^{d} R\left|\phi_k\right\rangle\left\langle\tilde{\phi}_k\right|$$
$$= R$$

3. A schematic model analysis

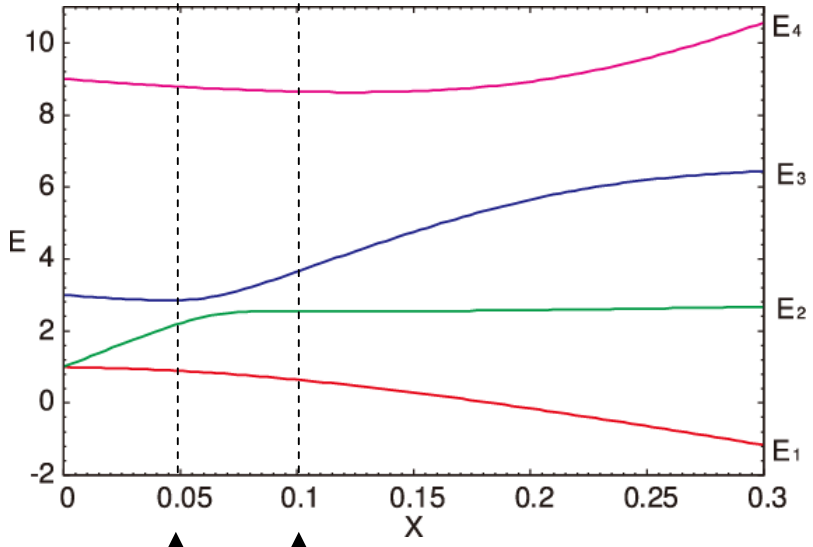
Modified Weidenmueler model Hamiltonian

[SOEK94]

$$H_0 \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 9 \end{pmatrix}, V \equiv \begin{pmatrix} 0 & 5x & -5x & 5x \\ 5x & 25x & 5x & -8x \\ -5x & 5x & -5x & x \\ 5x & -8x & x & -5x \end{pmatrix}$$

X: coupling strength

Its exact solution



Comparison with results of effective interaction

Model-space dimension d=2

$$E_0 = 1$$

$$PVP = \begin{pmatrix} 0 & 5x \\ 5x & 25x \end{pmatrix}, PVQ = \begin{pmatrix} -5x & 5x \\ 5x & -8x \end{pmatrix}, QVP = \begin{pmatrix} -5x & 5x \\ 5x & -8x \end{pmatrix}$$

$$QHQ = \begin{pmatrix} 3-5x & x \\ x & 9-5x \end{pmatrix}.$$

Methods for numerical calculation

1.KK method

$$[E_0 + \hat{Q}(E)]\left|\phi_k\right\rangle = G_k(E)\left|\phi_k\right\rangle, (k = 1, 2)$$

$$G_k(E): \text{eigen value of } E_0 + \hat{Q}(E); \quad G_1(E) < G_2(E)$$

If

$E=G_k(E)\cdots(1)$,

then E is a true eigen value.

Iteration equation $E^{(n+1)} = G_k(E^{(n)})$

2. EKK method

$$\hat{Z}(E) \equiv \frac{1}{1-\hat{Q}_1(E)}\left[\hat{Q}(E) - (E - E_0)\hat{Q}_1(E)\right] \cdots (2)$$

$$\left\{E_0 + \hat{Z}(E)\right\}\left|\phi_k\right\rangle = H_k(E)\left|\phi_k\right\rangle, (k = 1, 2) \cdots (3)$$

$$H_k(E): \text{eigen value of } E_0 + \hat{Z}(E); \quad H_1(E) < H_2(E)$$

If E is a solution to (1),

then E is also a solution to $E=H_k(E)$.$\cdots$(4)

Iteration equation $E^{(n+1)} = H_k(E^{(n)})$

In Newton-Raphson method

$$x_{n+1} = \frac{F(x_n) - x_n F'(x_n)}{1 - F'(x_n)}$$

For when $x_{n+1} = x_n = F(x_n)$, then we have

$F'(x_n) = 0 \longrightarrow$ Fast convergence

Therefore we have

$$\frac{d\hat{Z}(E)}{dE} = 0, \quad \frac{dH_k(E)}{dE} = 0 \quad \text{if } E \text{ is a solution.}$$

If G_k(E) has a pole, then $\hat{Q}_1(E)$ has a dominant contribution. Resultantly Z(E) becomes

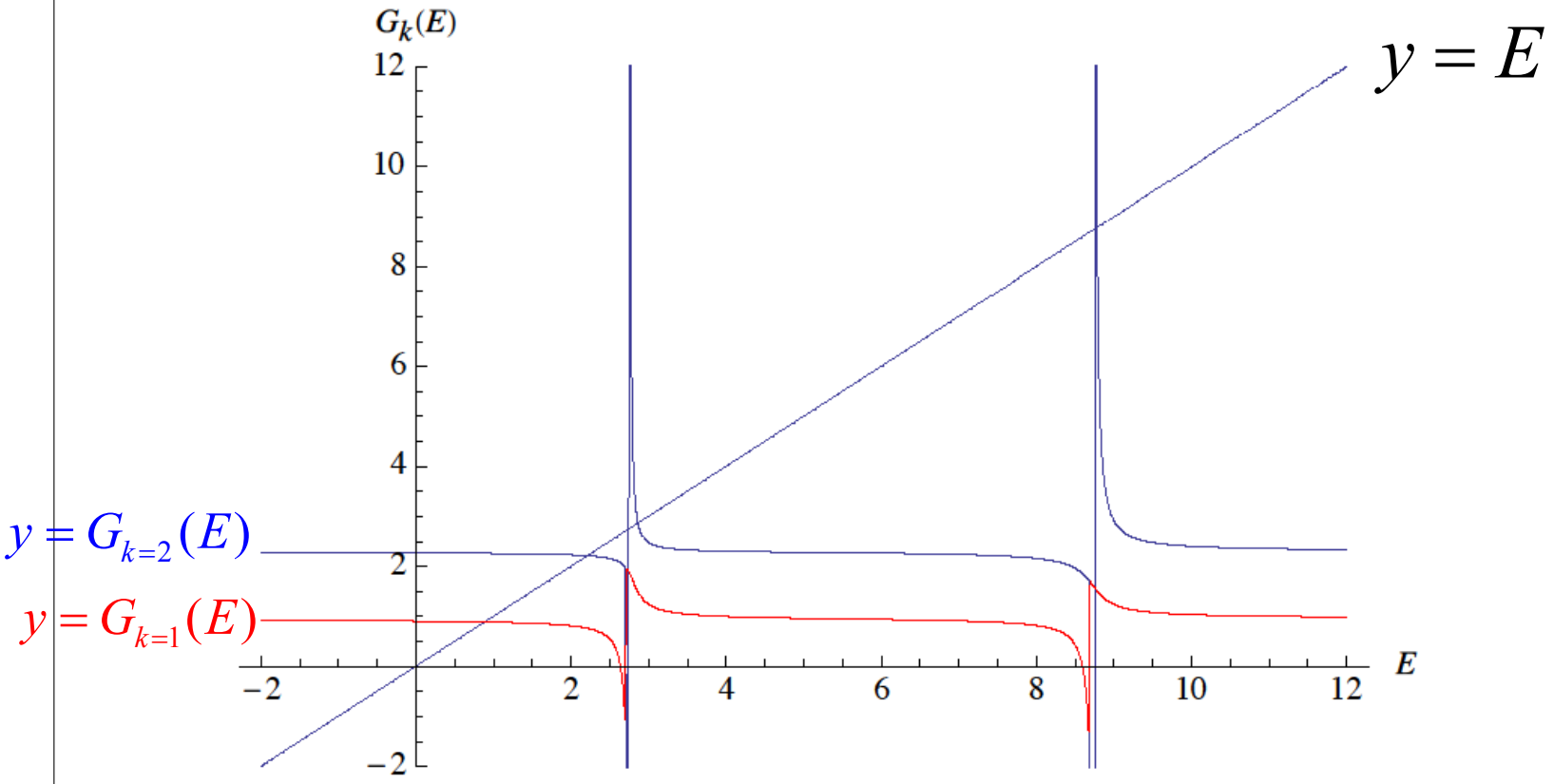
$$\hat{Z}(E) \equiv \frac{1}{1 - \hat{Q}_1(E)} \left[\hat{Q}(E) - (E - E_0)\hat{Q}_1(E) \right]$$

$$\approx (E - E_0)P$$

$G_k(E)$ (Krenciglowa-Kuo method)

*** Precision =30
*** x= 0.05
*** ncmax =1000
***(Emin, Emax) =-2. 12.

Near the pole positions → iteration is impossible



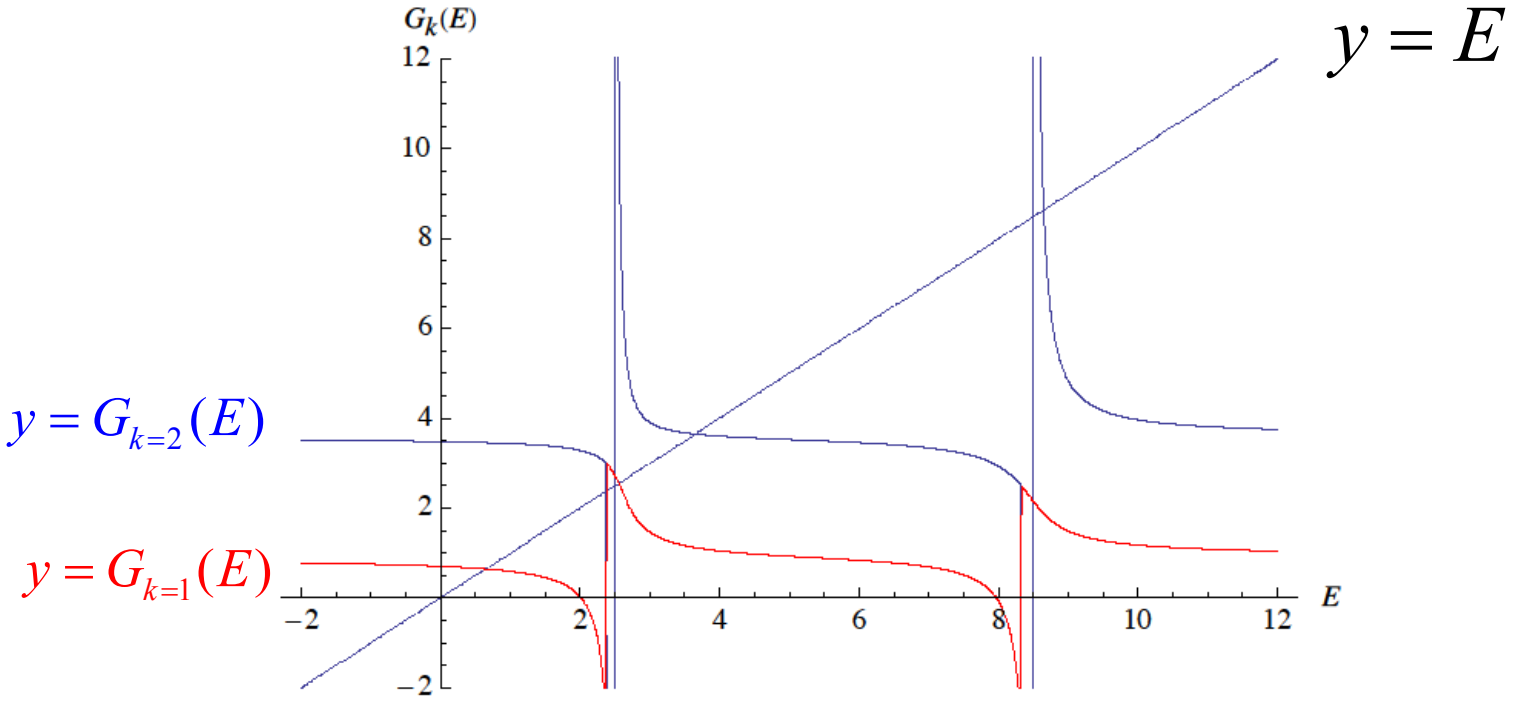
2010年5月15日土曜日

$G_k(E)$

(Krenciglowa-Kuo method)

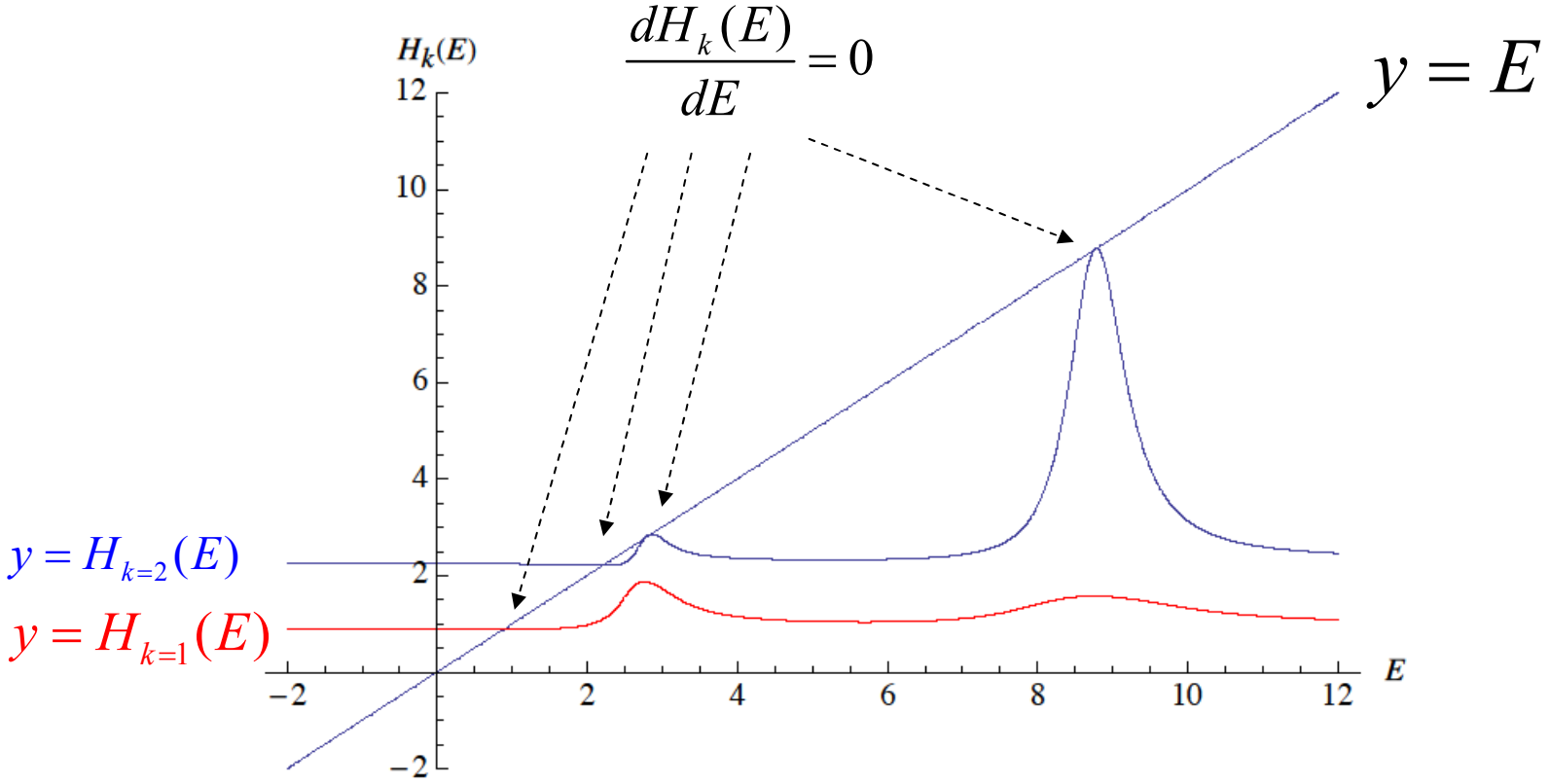
*** Precision =30
*** x= 0.10
*** ncmax =1000
***(Emin, Emax) =-2. 12.

Near the pole positions → iteration is impossible



$H_k(E)$ (Extended Krenciglowa-Kuo method)

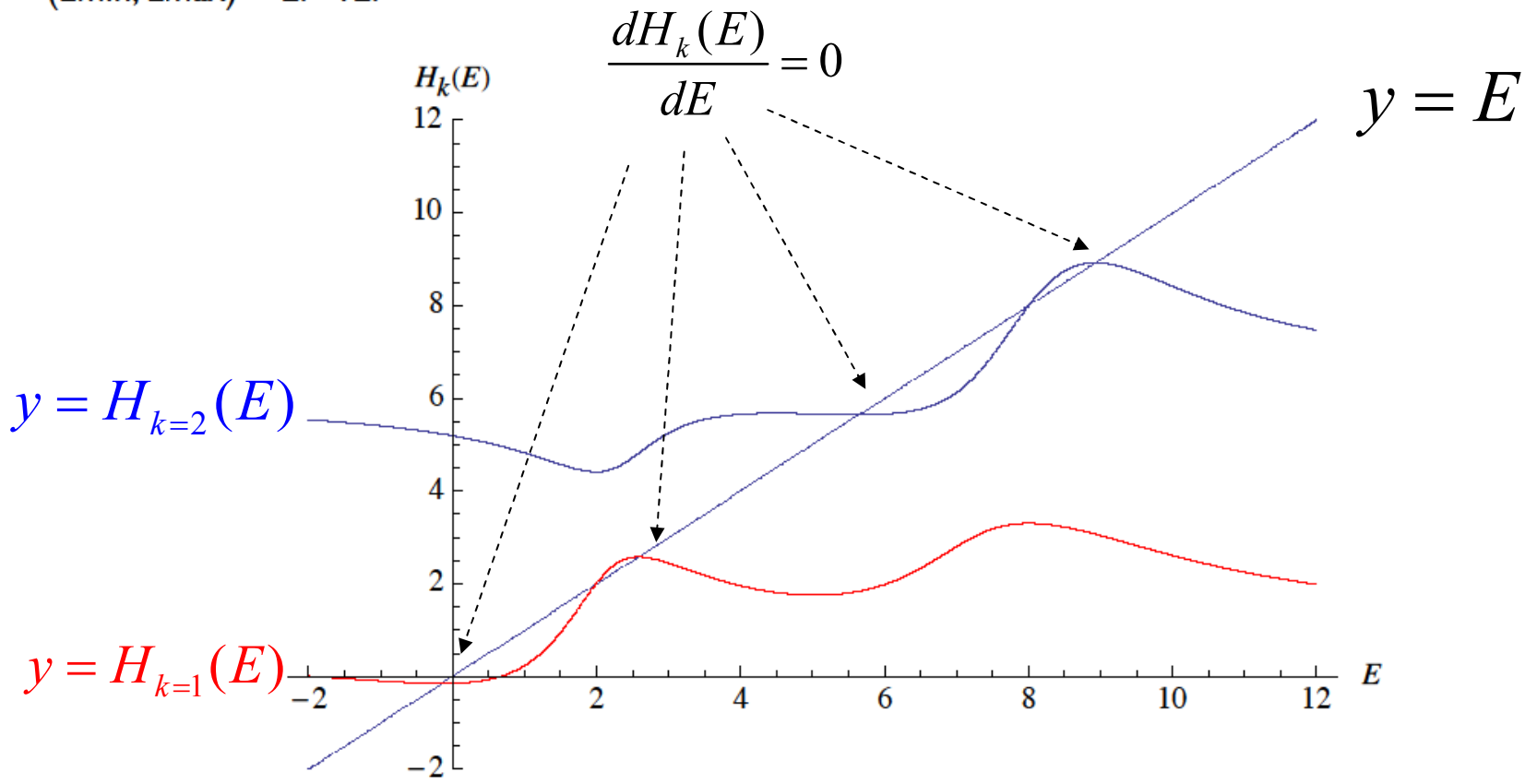
*** Precision =30
*** x= 0.05
*** ncmax =1000
***(Emin, Emax) = -2. 12.



$H_k(E)$

(Extended Krenciglowa-Kuo method)

*** Precision =30
*** x= 0.2
*** ncmax =1000
***(Emin, Emax) =-2. 12.



Calculated results(1) for x=0.05

1. KK method for x=0.05

Solutions converge to *largest P space* overlap (POV) states(E_1 *and* E_2) by choosing various initial energies, but not to E_3, E_4.

```
 *** K-K method ***
  *** Lower-energy solution ***
  ** starting energy=  0.000000000000000E+000
   n= 1  enew=     0.907650414522707   error= 0.1720D-01   elog= -1.7645
   n= 2  enew=     0.889961945687210   error= 0.4885D-03   elog= -3.3111
   n= 3  enew=     0.890464234309266   error= 0.1375D-04   elog= -4.8617
   n= 4  enew=     0.890450098879783   error= 0.3870D-06   elog= -6.4123
   n= 5  enew=     0.890450496780861   error= 0.1089D-07   elog= -7.9628
   n= 6  enew=     0.890450485580343   error= 0.3067D-09   elog= -9.5134
  n= 7  enew=     0.890450485895626   error= 0.8633D-11   elog=-11.0638
  n= 8  enew=     0.890450485886751   error= 0.2421D-12   elog=-12.6141
```

$\Leftrightarrow E_1^{\text{exact}}$

```
*** Upper-energy solution ***
 ** starting energy=  0.000000000000000E+000
 n= 1  enew=     2.270783708503062   error= 0.5510D-01   elog= -1.2588
n= 5  enew=     2.215689188920383   error= 0.8374D-05   elog= -5.0771
n= 6  enew=     2.215679904335437   error= 0.9107D-06   elog= -6.0406
 n= 7  enew=     2.215680914045184   error= 0.9904D-07   elog= -7.0042
n= 8  enew=     2.215680804239493   error= 0.1077D-07   elog= -7.9678
  n= 9  enew=     2.215680816180853   error= 0.1171D-08   elog= -8.9313
n=10  enew=     2.215680814882231   error= 0.1274D-09   elog= -9.8949
n=11  enew=     2.215680815023456   error= 0.1386D-10   elog=-10.8584
n=12  enew=     2.215680815008098   error= 0.1503D-11   elog=-11.8228
n=13  enew=     2.215680815009768   error= 0.1674D-12   elog=-12.7736
```

$\Leftrightarrow E_2^{\text{exact}}$

2. EKK method for x=0.05

Solutions converge to (E_1, E_2, E_3), *much more faster than KK method* by choosing various initial energies, but not to E_4.

```
 *** LSNR method ***
 *** Lower-energy solution ***
 ** starting energy=  0.000000000000000E+000
 n= 1  enew=    0.895660350298540   error= 0.5210D-02   elog= -2.2832
 n= 2  enew=    0.890450868550513   error= 0.3827D-06   elog= -6.4172
 n= 3  enew=    0.890450485886996   error= 0.2998D-14   elog=-14.3982
```

E_1^{exact}

```
 *** Upper-energy solution ***
 ** starting energy=  0.000000000000000E+000
 n= 1  enew=    2.256579157519787   error= 0.4090D-01   elog= -1.3883
 n= 2  enew=    2.216028537531382   error= 0.3477D-03   elog= -3.4588
 n= 3  enew=    2.215680836813825   error= 0.2180D-07   elog= -7.6615
 n= 4  enew=    2.215680815009604   error= 0.3109D-14   elog=-14.3863
```

E_2^{exact}

```
 ** starting energy=   3.00000000000000
 n= 1  enew=    2.763290145934360   error= 0.9887D-01   elog= -1.0049
 n= 2  enew=    2.775510759131921   error= 0.8665D-01   elog= -1.0622
 n= 3  enew=    2.795962996315704   error= 0.6620D-01   elog= -1.1792
 n= 4  enew=    2.824139100439752   error= 0.3802D-01   elog= -1.4200
 n= 5  enew=    2.850057431089997   error= 0.1210D-01   elog= -1.9171
 n= 6  enew=    2.860989025509985   error= 0.1172D-02   elog= -2.9311
 n= 7  enew=    2.862150194240400   error= 0.1074D-04   elog= -4.9689
 n= 8  enew=    2.862160935263002   error= 0.9003D-09   elog= -9.0456
 n= 9  enew=    2.862160936163269   error= 0.0000D+00   elog=-15.0000
```

E_3^{exact}

Calculated results(2) for x=0.10

1. KK method for x=0.10

Solutions converge to *largest-POV states(E_1 and E_3)* by choosing various initial energies, but not to E_2, E_4.
Slower than for x=0.05.

```
 *** K-K method ***
 *** Lower-energy solution ***
 ** starting energy=  0.000000000000000E+000
n= 1  enew=     0.706473608900947   error= 0.5822D-01   elog= -1.2349
n= 3  enew=     0.649118418572271   error= 0.8682D-03   elog= -3.0614
n= 5  enew=     0.648262842106936   error= 0.1260D-04   elog= -4.8997
n= 7  enew=     0.648250426803588   error= 0.1827D-06   elog= -6.7382
n= 9  enew=     0.648250246717693   error= 0.2651D-08   elog= -8.5767
n=11  enew=     0.648250244105535   error= 0.3845D-10   elog=-10.4151
n=13  enew=     0.648250244067645   error= 0.5579D-12   elog=-12.2527
```

E_1^{exact}

```
** starting energy=   3.00000000000000
n= 1  enew=     3.912285838536374   error= 0.2622D+00   elog= -0.5814
n= 3  enew=     3.656207627821902   error= 0.6097D-02   elog= -2.2149
n= 5  enew=     3.650276086634456   error= 0.1655D-03   elog= -3.7812
n= 7  enew=     3.650115108480489   error= 0.4510D-05   elog= -5.3458
n= 9  enew=     3.650110721206296   error= 0.1229D-06   elog= -6.9103
n=11  enew=     3.650110601622482   error= 0.3351D-08   elog= -8.4748
n=13  enew=     3.650110598362978   error= 0.9133D-10   elog=10.0394
n=15  enew=     3.650110598274134   error= 0.2489D-11   elog=-11.6038
 n=16  enew=    3.650110598271234   error= 0.4112D-12   elog=-12.3849
 *** Iteration converge ***
```

E_3^{exact}

2. EKK method for x=0.10

Solutions converge to (E_1, E_3), *much more faster than KK method,* by choosing various initial energies, but not to E_2, E_4.

```
*** LSNR method ***
 *** Lower-energy solution ***
 ** starting energy=  0.000000000000000E+000
n= 1  enew=     0.661722796801053   error= 0.1347D-01   elog= -1.8706
n= 2  enew=     0.648260424057093   error= 0.1018D-04   elog= -4.9923
n= 3  enew=     0.648250244072825   error= 0.5738D-11   elog=-11.2412
n= 4  enew=     0.648250244067087   error= 0.1110D-15   elog=-14.9543

*** Upper-energy solution ***
 ** starting energy=  0.000000000000000E+000
n= 1  enew=     3.393469129420620   error= 0.2566D+00   elog= -0.5907
n= 2  enew=     3.639581862233546   error= 0.1053D-01   elog= -1.9776
n= 3  enew=     3.650098978497770   error= 0.1162D-04   elog= -4.9348
n= 4  enew=     3.650110598257730   error= 0.1392D-10   elog=-10.8565
n= 5  enew=     3.650110598271645   error= 0.0000D+00   elog=-15.0000
```

E_1^{exact}

E_3^{exact}

4. Summary

In general one cannot control the convergence of the iterative solutions for a non-linear equation.

The iteration method does not work under the presence of poles.

The graphs of $G_k(E)$ and $H_k(E)$ give us important information for solving problems.

Focusing the local point, solve precisely by using non-iterative method, for example, bisection section method.

EKK method leads in general to much more faster convergence than KK method, and yield all solutions by choosing initial energy.

EKK method has some merits of both of previous methods, KK and LS.

References

[KK74] E. M. Krenciglowa and T. T. S. Kuo, Nucl. Phys. **A235**, 171 (1974).
[**LS80]** S. Y. Lee and K. Suzuki, Phys. Lett. **B91**, 173 (1980).
[SL80] K. Suzuki and S. Y. Lee, Prog. Theor. Phys. **64**, 2091 (1980).
[**SOEK94]** K. Suzuki, R. Okamoto, P. J. Ellis and T. T. S. Kuo,
Nucl. Phys. **A567**, 570 (1994).
[Andr96] F. Andreozzi, Phys. Rev. **C54**, 684 (1996).

Grazie per la vostra attenzione.

Thank you for your attention.