Spectral density for a discretized continuum

O.A. Rubtsova, V.N. Pomerantsev

Skobeltsyn Institute of Nuclear Physics, Moscow State University

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L^2 discretization

$$H\,|\Psi\rangle = E\,|\Psi\rangle$$

Expansion of the w.f. over some basis: $|\Psi\rangle = \sum_{n=1}^{N} C_n\,|\phi_n\rangle,\ \langle\phi_n|\phi_k\rangle = I_{nk}$

The eigenvalue problem: $\det \| H_{nn'} - E I_{nn'} \| = 0$

Discrete set of energies:

Unperturbed Hamiltonian H_0: $\left\{E_j^0\right\},\ j = 1,\ldots,N$

Total Hamiltonian $H = H_0 + V$: $\left\{E_j\right\},\ j = 1,\ldots,N$

The main question: How to extract scattering information from discrete eigenvalues representing continuum.

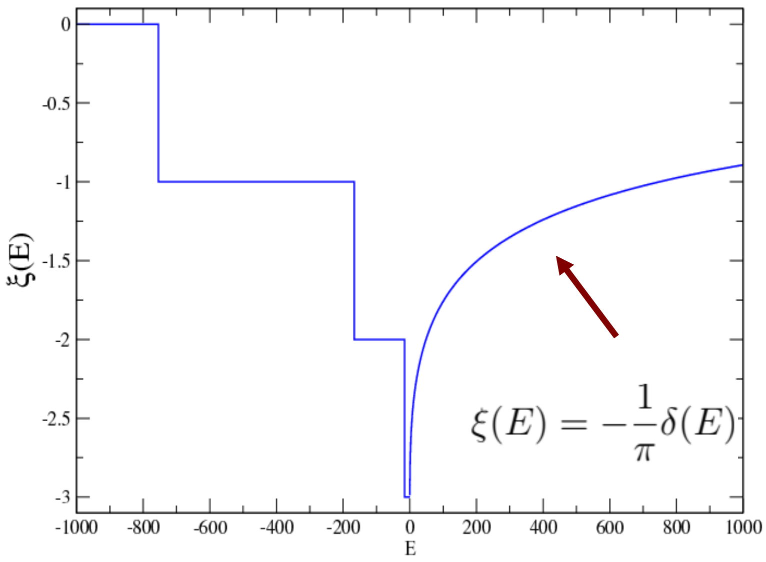
Spectral shift function

The spectral shift function corresponds to a pair of operators H_0 and $H=H_0+V$:

$$\mathrm{Tr}\left[F(H)-F(H_0)\right]=\int_{-\infty}^{\infty}F'(E)\xi(E)dE$$

the trace formula

Relation to S-matrix: $\det S(E)=\exp(-2\pi i\xi(E)) \Rightarrow \delta(E)=-\pi\xi(E)$



Spectral shift function for a model
Hamiltonian with 3 bound states

Spectral density

Spectral density for a Hamiltonian with discrete spectrum:

$$\rho_b(E) = \mathrm{Tr}\left[\delta(E - H_d)\right] = \sum_{n=1}^{N_b} \delta(E - E_n) \quad , E_n - \text{eigen energies}$$

Continuum level density:

$$\Delta(E) = -\frac{1}{\pi}\mathrm{Tr}\left\{\mathrm{Im}\left[E + i0 - H\right]^{-1} - \mathrm{Im}\left[E + i0 - H_0\right]^{-1}\right\}$$

'Naive' definition:

$$\Delta(E) = \mathrm{Tr}\left[\delta(E - H) - \delta(E - H_0)\right] \Leftrightarrow \rho(E) - \rho_0(E)$$

Relation to the SSF and phase shift ϕ:

$$\Delta(E) = -\frac{d\xi(E)}{dE} \qquad \left(\Delta(E) = \frac{1}{\pi}\frac{d\phi(E)}{dE}\right)$$

Thus, the SSF can be considered as integrated continuum level density:

$$\xi(E) = -\int_{-\infty}^{E} \Delta(E')dE'$$

$\Delta(E)$ includes a bound-state contribution.

Discretized continuum

Separate spectral densities can be defined:

$$\rho_{0d}(E) = \sum_{j=1}^{N} \delta\left(E - E_j^0\right) \quad \text{for } H_0 \text{ and} \quad \rho_d(E) = \sum_{j=1}^{N} \delta\left(E - E_j\right) \quad \text{for } H$$

Integrated densities of states (IDS):

$$J_0(E) = \int_{-\infty}^{E} \rho_{0d}(E')dE' = \sum_{j=1}^{N} \theta\left(E - E_j^0\right), \quad J_0\left(E_j^0\right) = j \qquad J(E) = \sum_{j=1}^{N} \theta\left(E - E_j\right), \quad J\left(E_j\right) = j$$

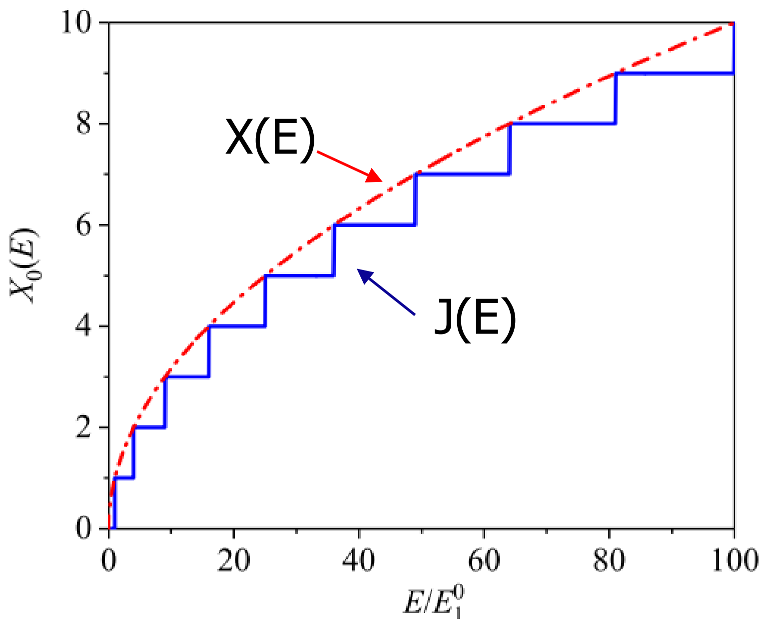
One may consider the differences:

$$\rho_d(E) - \rho_{0d}(E) \;\rightarrow\; \Delta(E)$$

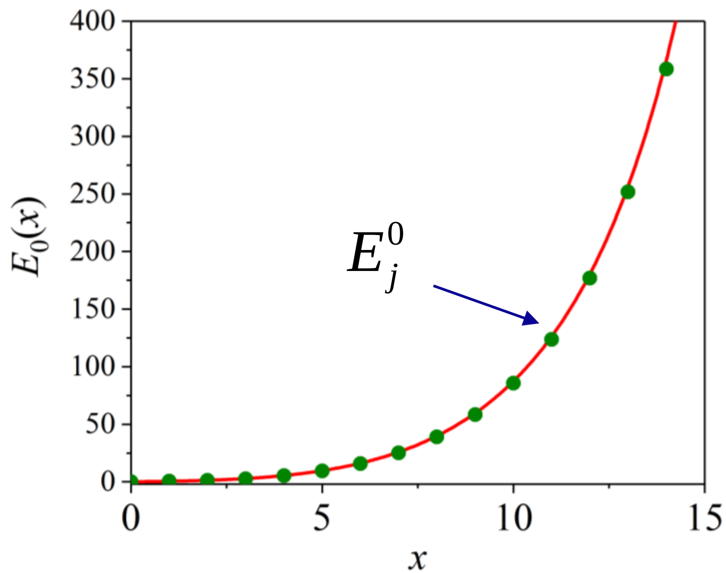
$$-\left[J(E) - J_0(E)\right] \;\rightarrow \xi(E)$$

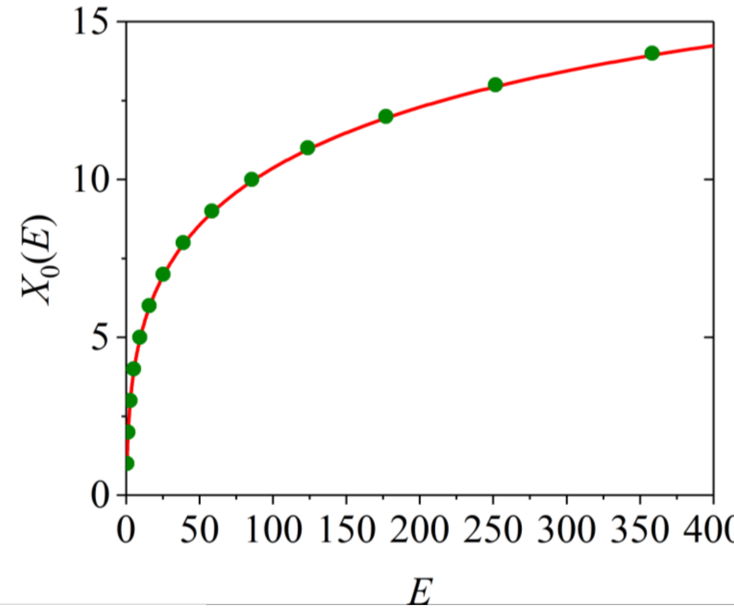
But they do not contain any information about scattering.

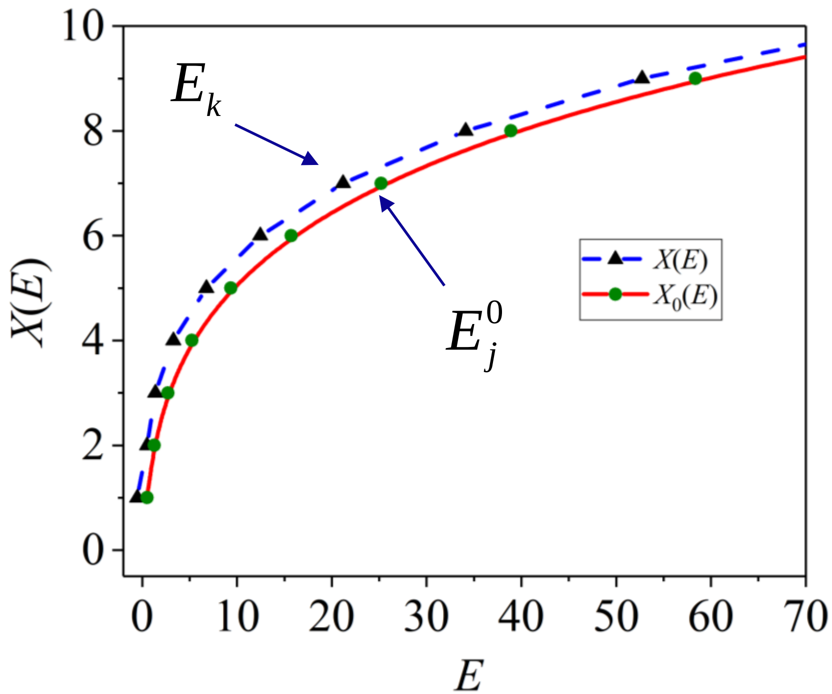
The main idea: to construct smooth functions instead of the step-like ones: $J(E) \rightarrow X(E)$.



IDS for the problem in a box







Difference of $X(E)$ and $X_0(E)$ would give the SSF (and the phase shift):

$$\xi(E) = -\left(X(E) - X_0(E) \right)$$

Quasi-continuous spectrum (I.M. Lifshits, 1947)

For the initial Hamiltonian H_0 with continuous spectrum, one considers a family of operators $H_0(\alpha)$ (α is a small parameter) with discrete spectra:

$$E_j^{0(\alpha)} = \lambda_0(j\alpha) + O(\alpha), \quad D_j^{(\alpha)} \equiv E_{j+1}^{0(\alpha)} - E_j^{0(\alpha)} = \alpha \left[\left. \frac{d\lambda_0(u)}{du} \right|_{u=j\alpha} + O(\alpha) \right]$$

- eigenvalues belong to some smooth monotonous function;
- one may consider a limit $\alpha \to 0$.

It has been shown by I.M. Lifshits, the EVs for the total Hamiltonian $H(\alpha)=H_0(\alpha)+V$ are related to EVs of unperturbed Hamiltonian:

the SSF

$$E_j^{(\alpha)} = E_j^{0(\alpha)} + \alpha \left. \frac{d\lambda_0(u)}{du} \right|_{u=j\alpha} \xi_j^{(\alpha)}, \qquad \xi_j^{(\alpha)} \to \xi(E_j)$$

Can be considered as the Taylor expansion: $E_j^{(\alpha)} = \lambda(\alpha j) \approx \lambda_0\left(\alpha\left[j + \xi_j\right]\right)$

Functions X_0 and X can be defined as an inverse functions:

$$\alpha X_0^{(\alpha)}(E) \equiv \lambda_0^{-1}(E) \qquad\qquad \alpha X^{(\alpha)}(E) \equiv \lambda^{-1}(E)$$

This leads to the same expression for the SSF via the integrated densities:

$$\alpha\left[X^{(\alpha)}(E) + \xi^{(\alpha)}(E)\right] = \lambda_0^{-1}(E) = \alpha X_0(E) \Rightarrow \quad \xi^{(\alpha)}(E) = -\left(X^{(\alpha)}(E) - X_0^{(\alpha)}(E)\right)$$

Spectral densities

The spectral shift function:

$$\xi^{(\alpha)}(E) = -\left(X^{(\alpha)}(E) - X_0^{(\alpha)}(E)\right)$$

and the phase shift:

$$\delta^{(\alpha)}(E) = \pi\left(X^{(\alpha)}(E) - X_0^{(\alpha)}(E)\right)$$

One can also define separate spectral densities:

$$\rho_0^{(\alpha)}(E) \equiv \frac{dX_0^{(\alpha)}(E)}{dE}, \qquad \rho^{(\alpha)}(E) \equiv \frac{dX^{(\alpha)}(E)}{dE},$$

and the CLD:

$$\Delta^{(\alpha)}(E) = \frac{dX^{(\alpha)}(E)}{dE} - \frac{dX_0^{(\alpha)}(E)}{dE}$$

The functions X, X_0 and ρ, ρ_0 do not correspond to initial spectra. They depend on the function λ_0. However, the limits for the functions ξ and Δ do exist, so one may expect that they will 'converge' to exact functions when $\alpha \longrightarrow 0$.

The properties of functions X and X_0

$$\delta^{(\alpha)}(E) = \pi\left(X^{(\alpha)}(E) - X_0^{(\alpha)}(E) \right)$$

$$X^{(\alpha)}(E_j) = j \longrightarrow \delta^{(\alpha)}(E_j) = \pi j - \pi X_0^{(\alpha)}(E_j), \quad j = n_b + 1, \ldots$$

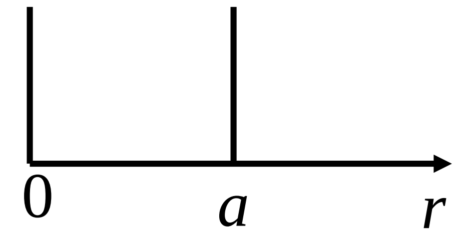
At the points of the total Hamiltonian's spectrum, the phase shifts are defined via the function X_0 only!

By using an expansion of X_0 at the point E_k^0 which is closest to E_j and

$$\frac{dX_0(E_k^0)}{dE} = \left[\frac{dE_0(x=k)}{dx} \right]^{-1} \approx \frac{1}{D_k}$$

$$\delta^{(\alpha)}(E_j) \approx \pi(j-k) + \pi \frac{E_k^0 - E_j}{D_k}$$

Scattering problem in a box



Discrete spectrum of the free Hamiltonian:

$$\sin(k_n^0 a) = 0 \Rightarrow k_n^0 = n\frac{\pi}{a}, \quad E_n^0 = \frac{1}{2m}\frac{\pi^2}{a^2}n^2, \quad n = 1, \ldots$$

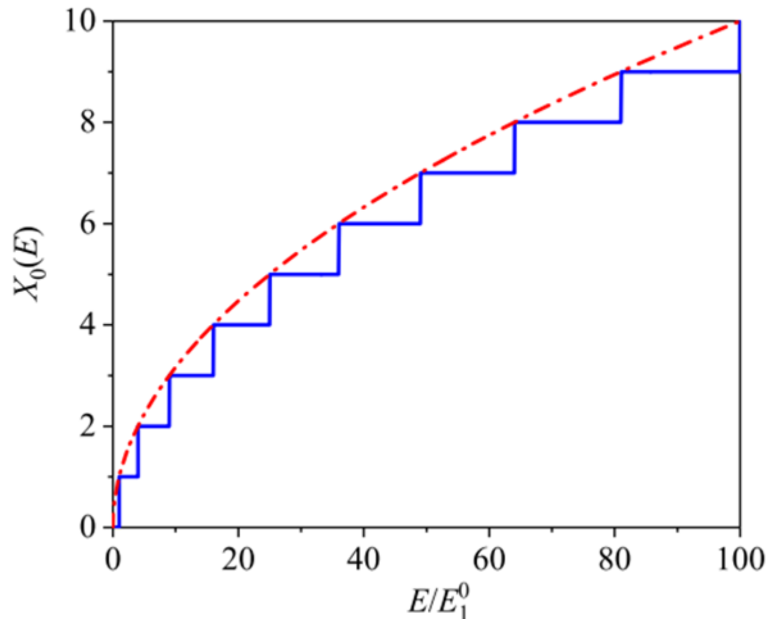
The small parameter: $\alpha \sim \frac{1}{a}$

Integrated density:

$$X_0^{(a)}(E) = \frac{a}{\pi}\sqrt{2mE}$$

The phase shift:

$$\delta^{(a)}(E_n) = -a\sqrt{2mE_n}, \quad n = n_b + 1, \ldots.$$



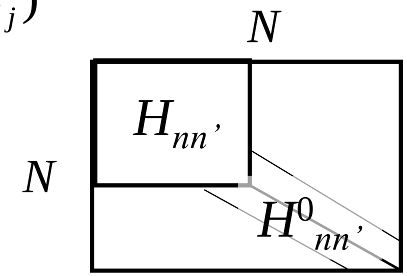
From the boundary condition:

$$\sin\left(a\sqrt{2mE_n} + \delta^{(a)}(E_n)\right) = 0$$

Cases when X_0 is known explicitly

$$\delta(E) = \pi\big(X(E) - X_0(E)\big) \quad \Rightarrow \quad \delta(E_j) = j\pi - \pi X_0(E_j)$$

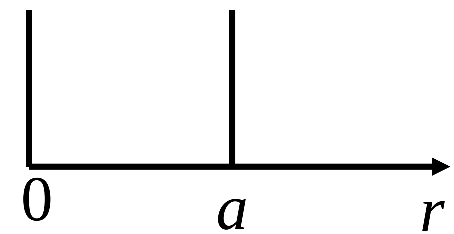
The J-matrix approach – the SS-HORSE method (A.M. Shirokov et al., PRC 2016):



$$\delta(E_{nl}) = f_{Nl}(E_{nl}), \quad f_{Nl}(E) \equiv -\tan^{-1}\frac{S_{N+1,l}(E)}{C_{N+1,l}(E)} \qquad X_0^{(N)}(E) = \frac{1}{\pi}\tan^{-1}\frac{S_{N+1,l}(E)}{C_{N+1,l}(E)}$$

The function $X(E)$ can be also calculated in the HORSE method.

In the R-matrix method: $\delta_l(E) = \eta_l(E) - \phi_l(E)$



$$\phi_l(E) = \tan^{-1}\frac{j_l(ka)}{n_l(ka)}, \quad k = \sqrt{2mE}$$ hard sphere phase shift

$$\delta^{(a)}(E_{nl}) = -\pi X_0^{(a)}(E_{nl}) = -\phi_l(E_{nl})$$

E_{nl} - energies of states for which R-matrix is diagonal

Within the both methods, the charged particle scattering can be considered as well.

Multiple Gaussian bases

Radial functions: $\varphi_j(r) = A_{jl} r^l \exp(-\beta_j r^2), \ \ j = 1, \ldots, N$

Scale parameters:

$$\beta_j = g_N(j), \ \ \beta_j = \beta_0 \left(\tan\left[\frac{j}{N+1} \frac{\pi}{2} \right] \right)^t$$

Eigenvalue problems for H_0 and H:

$$\det \| H_{nn'} - E I_{nn'} \| = 0 \rightarrow \left\{ E_j^0 \right\}_{j=1}^N \ \left\{ E_j \right\}_{j=1}^N$$

Consider a set of M bases with shifted scale parameters:

$$\left[\beta_j^m = g_N \left(j + a_m - 1 \right), \, j = 1, \ldots, N \right]_{m=1}^M, \ \ 0 < a_1 < \ldots < a_M < 1$$

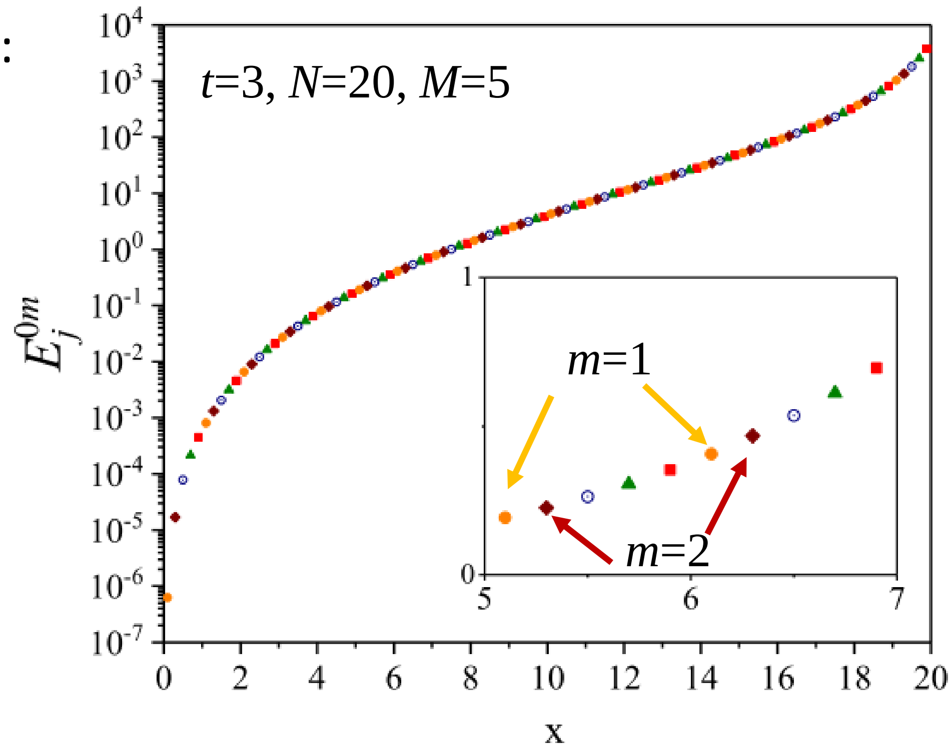
This imitates continuous dependence:

$$\beta(x) = g_N(x), \ \ 0 < x \le N$$

The eigenvalues (found from M eigenvalue problems) have the similar property - dependence on common index x:

$$E_j^{0m} = \lambda_0(x\alpha), \ \ x = j + a_m - 1$$

$$\alpha \sim \frac{1}{N+1}$$



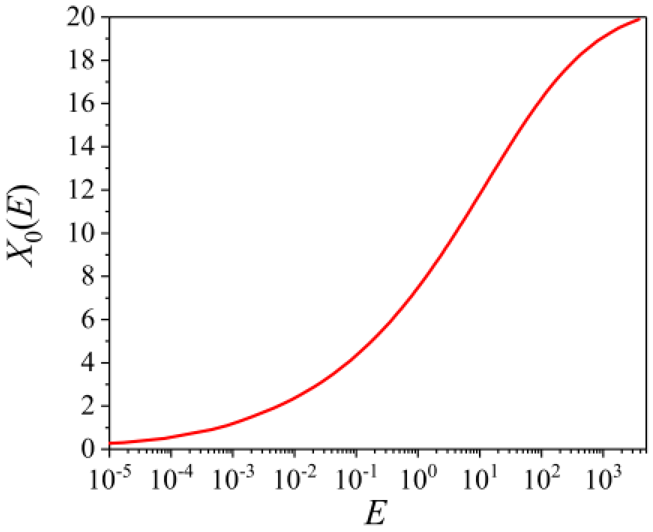
Case of non-integer indices

Thus one can construct the ISD as follows:

$$X_0^{(N)}\left(E_j^{0m}\right) = j + a_m - 1, \quad j = 1,\ldots,N, \quad m = 1,\ldots,M$$

(to be compared with $X_0^{(N)}\left(E_j^{0}\right) = j$)

Integrated density of states reconstructed from 20 Gaussian bases →



The same procedure for the spectrum of H:

$$X^{(N)}\left(E_k^{m}\right) = k + a_m - 1$$

The generalized relation for the phase shift:

$$\delta^{(N)}\left(E_k^{m}\right) = \pi\left[k + a_m - 1 - X_0^{(N)}\left(E_k^{m}\right)\right], \quad 1 \le k \le N, \quad 1 \le m \le M$$

Numerical examples

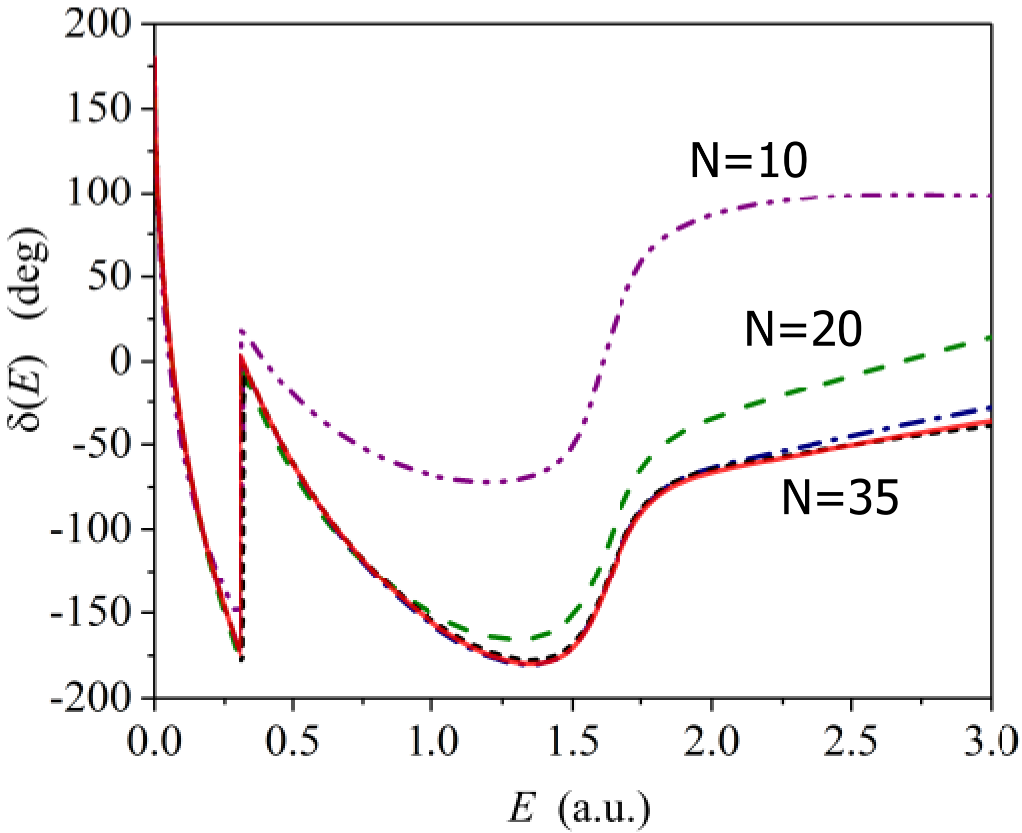
$$H_0 = T, \quad H = H_0 + V$$

(Csoto et al., PRA 1990)

$$V(r) = -8\exp(-0.16r^2) + 4\exp(-0.04r^2),$$

atomic units

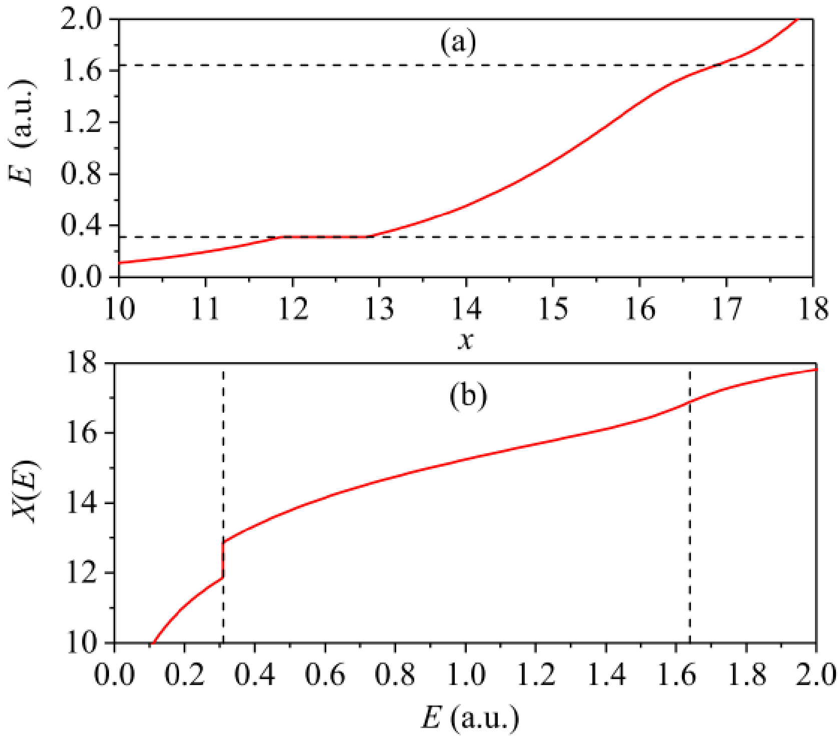
orbital momentum L=0



Direct solution of Schroedinger eq.

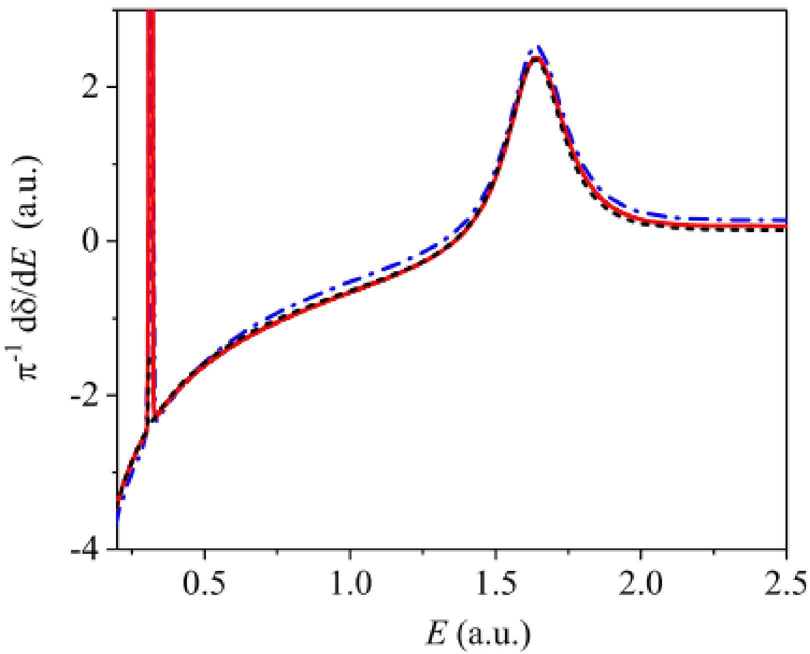
There is one bound state, and two resonances for this potential.

$E(x)$ has a 'plato' in the resonance region similarly to the stabilization approach



Continuum level density:

$$\Delta(E) = \frac{1}{\pi}\frac{d\delta(E)}{dE}$$



The second resonance:

E_R=1.64 a.u., Γ= 0.27 a.u.

(pole position: E=1.632 – i 0.123 a.u. [H.A. Yamani, 1993])

Case of narrow resonance

$$\Delta(E) = \frac{1}{\pi}\frac{d\delta(E)}{dE} \approx \frac{1}{\pi}\frac{\Gamma/2}{(E-E_R)^2+\Gamma^2/4}$$

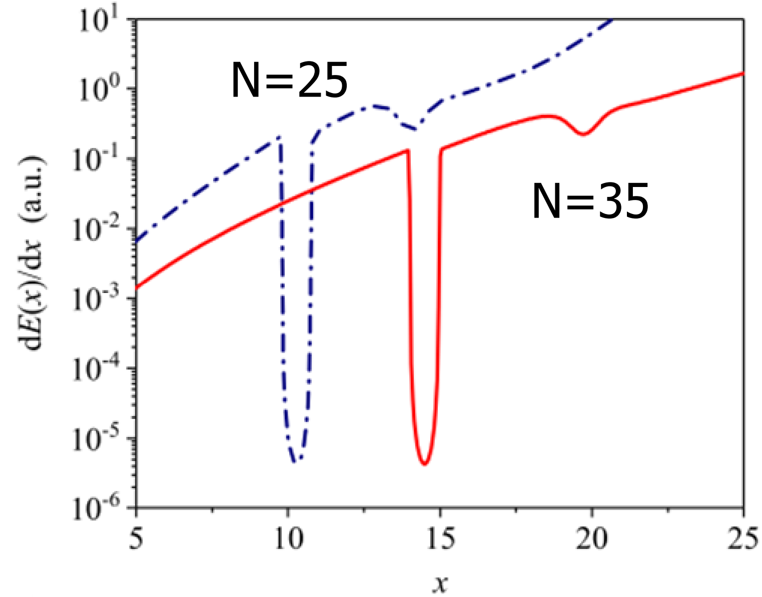
The phase shift changes rapidly on the interval of energies $\sim\Gamma$

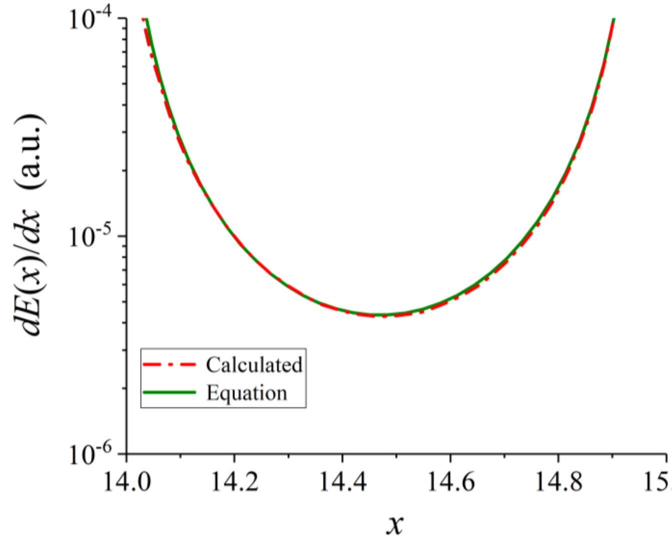
$$\frac{1}{\pi}\frac{d\delta(E)}{dE} \approx \frac{dX(E)}{dE}$$

$$\frac{dE(x)}{dx} \approx \pi \frac{\Gamma/2}{\cos^2 \pi(x-x_R)}$$

The shape does not depend on Γ

E_R=0.31009 a.u., Γ= $3\cdot10^{-6}$ a.u.



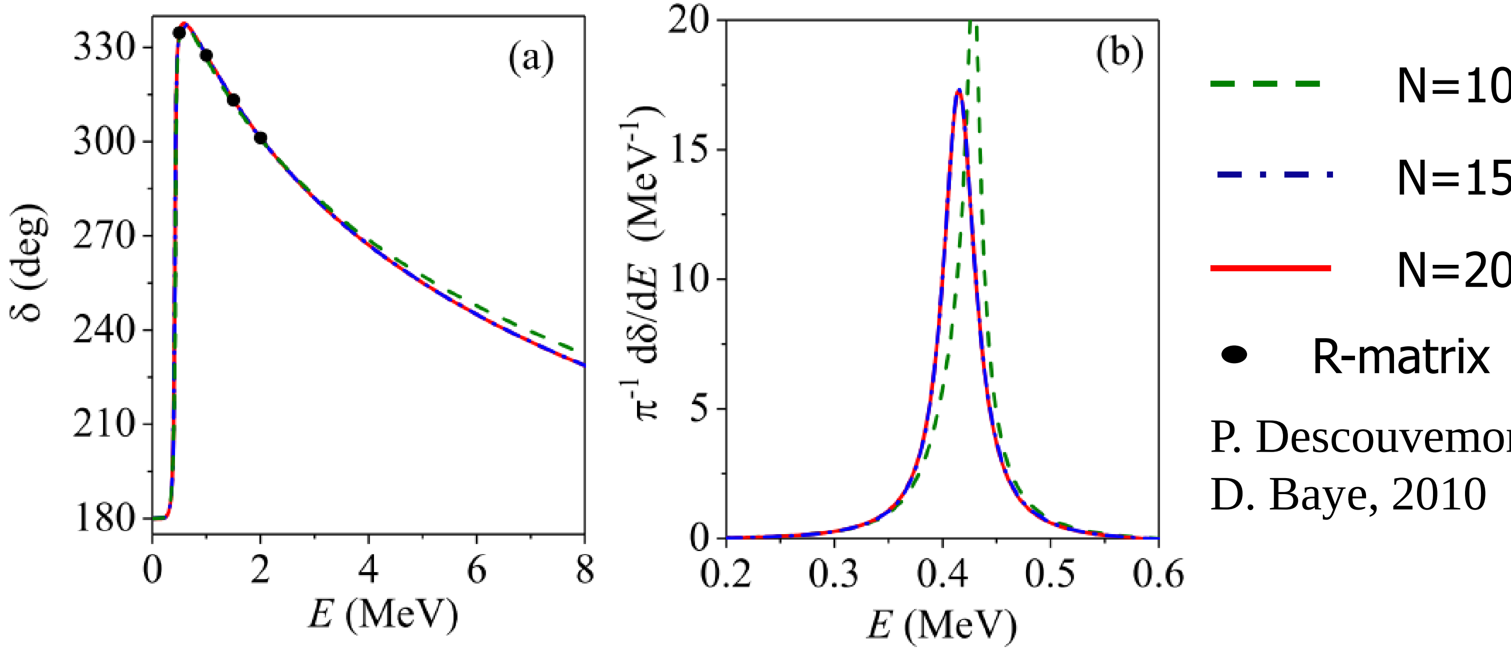


$p+^{12}C$ scattering

Unperturbed Hamiltonian includes Coulomb interaction:

$$H_0 = T + \frac{6e^2}{r}$$

Short-range nuclear potential: $V(r) = V_0 \exp(-(r/r_0)^2)$, L=0



P. Descouvemont, D. Baye, 2010

There is one forbidden state

$E_R = 0.415$ MeV and $\Gamma = 37$ keV

Coupled channel scattering

Total Hamiltonian: $H_{\nu\nu'} = H_{0\nu}\delta_{\nu\nu'} + V_{\nu\nu'}, \quad \nu,\nu' = 1,\ldots,N$

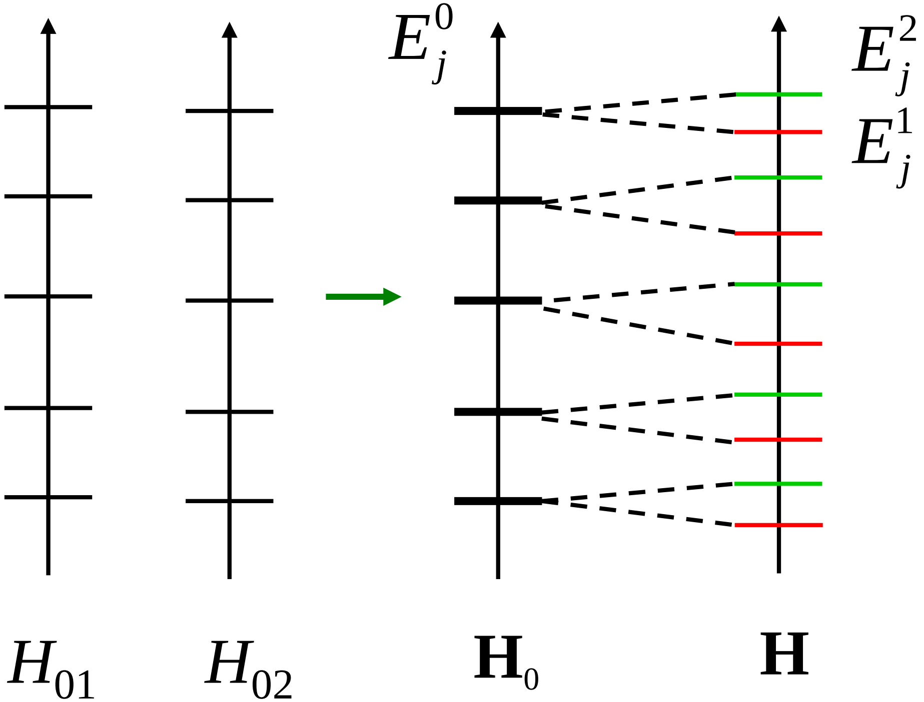
It has been shown (O.A.R., V.N.P. et al. PRC 2010) that if the discretized spectrum of $\mathbf{H_0}$ is degenerated then one can divide the discretized spectrum of the total Hamiltonian $\mathbf{H}$ into different branches corresponding to the eigen channels of scattering.

In such a case functions $X_0(E)$ are the same for each channel.

By collecting energies from each branch one can reconstruct functions $X_\nu(E)$.

The eigen phases can be found from differences:

$$\delta_\nu(E) = \pi\left(X_\nu(E) - X_0(E)\right)$$



However, the question how to reconstruct X in a general case (without a degeneracy of the unperturbed discretized spectrum) is still open.

Summary

- The formalism with smooth spectral densities and integrated densities has been introduced for discretized continuum.
- Spectral shift function formalism is quite suitable for studying discretized spectrum within different approaches.
- The multiple bases of Gaussians (MBG) allow to work with much more dense discretized spectrum.

Further development

- Multi-channel problem for non-degenerated discretized spectrum.
- The MBG might be useful for three- and few-body scattering calculations within approaches which employ integral equation formalism.

Talk of M.N. Platonova: Dibaryon resonances and three-body forces in large-angle pd scattering at intermediate energies
Friday, Section 1, 15:20

Thank you for your attention!