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SPRING COLLEGE ON AMORPHOUS SOLIDS
AND THE LIQUID STATE

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SMALL POLARON CONDUCTION

(Lecture III)

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Bargmann Hilbert space of analytical functions

$$H = \hbar\omega_0 a^+ a$$

$$|n\rangle = \frac{a^{+n}}{\sqrt{n!}}|0\rangle \quad \to \quad z^n \frac{1}{\sqrt{n!}} ;$$

$$a^+ \to z \qquad \left(\frac{d}{dz} z - z\frac{d}{dz}\right) f(z) = f(z)$$

$$a \to \frac{d}{dz}$$

$$\langle m|n\rangle = \frac{1}{\pi}\int d\mathrm{Re}\,z \int d\mathrm{Im}\,z \; e^{-zz^*} \frac{z^{*m}}{\sqrt{m!}} \frac{z^n}{\sqrt{n!}}$$

$$= \frac{1}{\pi}\int dR \int d\varphi \; e^{-R^2} R \frac{R^{m+n}}{\sqrt{m!}\sqrt{n!}} e^{+i(n-m)\varphi}$$

$$= \delta_{m,n}$$

$$H\psi(z) = E\psi(z)$$

$$\hbar\omega_0 z\frac{d}{dz}\psi(z) = E\psi(z)$$

$$\frac{d\psi}{\psi} = \frac{E}{\hbar\omega_0}\frac{dz}{z}$$

$$\psi = z^{\frac{E}{\hbar\omega_0}} \qquad \rightsquigarrow \quad E = n\hbar\omega_0$$

D.H.O.

$$\left\{\hbar\omega_0 z\frac{d}{dz} + \hbar\chi\left(z+\frac{d}{dz}\right)\right\}\psi = E\psi$$

$$\left(\hbar\omega_0 z + \hbar\chi\right)\frac{d}{dz}\psi = \left(E - \hbar\chi z\right)\psi$$

$$\frac{d\psi}{\psi} = \frac{E-\hbar\chi z}{\hbar\omega_0 z + \hbar\chi}\, dz$$

$$\frac{d\psi}{\psi} = \frac{E - \hbar\chi\left(z+\frac{\hbar\chi}{\hbar\omega_0}\right) + \frac{\hbar\chi^2}{\omega_0}}{\hbar\omega_0\left(z+\frac{\hbar\chi}{\hbar\omega_0}\right)}\, dz$$

$$= \left(\frac{E+\hbar\chi^2/\omega_0}{\hbar\omega_0\left(z+\frac{\hbar\chi}{\hbar\omega_0}\right)} - \chi/\omega_0\right) dz$$

$$\psi = e^{-\chi/\omega_0 z}\left(z+\frac{\chi}{\omega_0}\right)^{\frac{E+\hbar\chi^2/\omega_0}{\hbar\omega_0}}$$

$$\rightsquigarrow \quad E = -\hbar\frac{\chi^2}{\omega_0} + n\hbar\omega_0$$

$$H = \hbar\omega_0\left(a^+_{(+)}a_{(+)} + a^+_{(-)}a_{(-)}\right) + \tfrac{1}{2}\hbar\Delta\sigma_z$$
$$+ \hbar k\left\{(a_{(+)} + a^+_{(-)})\sigma_{(+)} + (a_{(-)} + a^+_{(+)})\sigma_{(-)}\right\}$$

$$\mathcal{J} = a^+_{(+)}a_{(+)} - a^+_{(-)}a_{(-)} + \tfrac{1}{2}\sigma_z$$

$$\Psi_{j+1/2}\rangle = a^{+j}_{(+)}\phi(a^+_{(+)}a^+_{(-)})|0\rangle\uparrow\rangle + a^{+j+1}_{(+)} f(a^+_{(+)}a^+_{(-)})|0\rangle|\downarrow\rangle$$

$$\mathcal{J}\Psi_{j+1/2}\rangle = (j+1/2)\Psi_{j+1/2}\rangle$$

$$\frac{H}{2\hbar\omega_0} = \tfrac{1}{2}\mathcal{J} + h_{(+)}$$

$$h_{(+)} = a^+_{(-)}a_{(-)} + \delta\sigma_z + \varkappa\left\{(a_{(+)} + a^+_{(-)})\sigma_{(+)} + (a_{(-)} + a^+_{(+)})\sigma_{(-)}\right\}$$

$$\delta = \frac{1}{4}\frac{\Delta - \omega_0}{\omega_0} \quad ; \quad \varkappa = \frac{k}{2\omega_0}$$

$$h_{(+)}\Psi\rangle_{j+1/2} = \varepsilon\,\Psi\rangle_{j+1/2} \qquad \lambda = 2\varepsilon + j + 3/2$$

Bargmann Fock $\quad a^+_{(+)} \to \xi \quad a_{(+)} = \frac{\partial}{\partial\xi}$

$\quad a^+_{(-)} \to \eta \quad a_{(-)} = \frac{\partial}{\partial\eta}$

$$\Psi_{j+1/2} = \xi^j\phi(z)\uparrow + \xi^{j+1}f(z) \qquad z = \xi\cdot\eta$$

$$h_{(+)} = \eta\frac{\partial}{\partial\eta} + \delta\sigma_z + \varkappa\left\{\left(\frac{\partial}{\partial\xi} + \eta\right)\sigma_{(+)} + \left(\frac{\partial}{\partial\eta} + \xi\right)\sigma_{(-)}\right\}$$

$$\eta\frac{\partial}{\partial\eta}\,\xi^j\phi(\xi\eta) = \eta\,\xi^j\frac{d}{dz}\phi(z)\cdot\xi = \xi^j\,z\frac{df}{dz}$$

$$z\frac{d\phi(z)}{dz} - (\varepsilon - \delta)\phi(z) + \varkappa\left\{z\frac{df}{dz} + (j+1+z)f(z)\right\} = 0$$

$$\varkappa\left\{\frac{d\phi}{dz} + \phi(z)\right\} + z\frac{df}{dz} - (\varepsilon + \delta)f(z) = 0$$

Small polaron

$$h = \frac{H}{\hbar\omega_0} = b^+b + \underset{\substack{\uparrow\\ \text{tunneling term}}}{(1/2 + 2\delta)\sigma_z} + \sqrt{2}\varkappa(b + b^+)\underset{\substack{\uparrow\\ \sigma_x}}{(\sigma_{(+)} + \sigma_{(-)})}$$

~~Ansatz 1~~ $\quad \cancel{\Psi_1 = \phi_1(\xi)} \qquad b^+ = \xi \qquad b = \frac{d}{d\xi}$

$$h = \xi\frac{d}{d\xi} + (1/2 + 2\delta)\sigma_z + \sqrt{2}\varkappa\left(\frac{d}{d\xi} + \xi\right)(\sigma_{(+)} + \sigma_{(-)})$$

Ansatz 1 $\quad \Psi_1 = \phi_1(\xi)\uparrow + \frac{1}{\sqrt{2}}\xi f_1(\xi)\downarrow$

$$\xi\frac{d\phi_1(\xi)}{d\xi} + (1/2 + 2\delta - \lambda)\phi_1(\xi) + \varkappa\left\{(\xi^2+1)f_1(\xi) + \xi\frac{df_1}{d\xi}\right\} = 0$$

$$\varkappa\left\{2\phi_1(\xi) + \frac{2}{\xi}\frac{df_1}{d\xi}\right\} + \xi\frac{df_1}{d\xi} + (-1/2 - 2\delta - \lambda)f_1 = 0$$

$$z = 1/2\,\xi^2 \qquad \lambda = 2\varepsilon + 1/2$$

$$z\frac{d\phi_1}{dz} - (\varepsilon - \delta)\phi_1(z) + \varkappa\left\{z\frac{df_1}{dz} + (1/2 + z)f_1(z)\right\} = 0$$

$$\varkappa\left\{\frac{d\phi_1}{dz} + \phi_1(z)\right\} + z\frac{df_1}{dz} - (\varepsilon + \delta)f_1(z) = 0$$

$$j = -1/2\ !$$

Ansatz 2 $\quad \psi_2 = \frac{1}{\sqrt{2}} \, \zeta \, \phi_2(\zeta)\uparrow + f_2(\zeta)\downarrow$

$$f_2(z,\delta) = \phi_1(z, -\delta - 1/2)$$
$$\phi_2(z,\delta) = f_1(z, -\delta - 1/2)$$

$$\phi(z) = \frac{\ell}{\varkappa^2} \sum_n \frac{\alpha_n}{n!\,\varkappa^{4n}} (\varkappa^2 z)^{(n-j)/2} I_{n+j}(2\varkappa z^{1/2})$$

$$f(z) = \frac{c}{\varkappa} \sum_n \frac{\beta_n}{n!\,\varkappa^{4n}} (\varkappa^2 z)^{(n-j-1)/2} I_{n+j+1}(2\varkappa z^{1/2})$$

$$\lambda = \frac{1}{2} + v - 2\varkappa^2$$

$$\begin{pmatrix} \alpha_{n+1} \\ \beta_{n+1} \end{pmatrix} = \begin{pmatrix} M_{11}(n+1,n) & M_{12}(n+1,n) \\ M_{21}(n+1,n) & M_{22}(n+1,n) \end{pmatrix} \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix}$$

$$\left.\begin{aligned} \alpha_0 &\sim \varkappa^2 \\ \beta_0 &= -\varkappa^2 - j/2 - 1/2 - \delta + v/2 . \end{aligned}\right\} \text{Sing pt } z=0$$

M_{11} etc rational fns of $\varkappa^2, v$ (j, δ)

$$\operatorname{Det} M(n+1,n) = -\varkappa^4 (n-v)(n+1)$$

$$\operatorname{Tr} M(n+1,n) = (j/2 + 3/2 + \delta + n - v/2)(j/2 + 1/2 - \delta + n - v/2) - \varkappa^2(v+1)$$

$$M_{11} = -\varkappa^2 (j/2 + 1/2 - \delta + v/2)$$

$$M_{12} = -\varkappa^2 (j/2 + 1/2 - \delta + n - v/2)$$

α_n, β_n are rational fns of $\varkappa^2, v$

$\alpha_n + \beta_n$ = Polynomial $(\varkappa^2)^n$

Take $v = n$; $\quad \operatorname{Det} M(n+1, v) = 0$

then $\left.\begin{aligned} \alpha_{n+m} &= 0 \\ \beta_{n+m} &= 0 \end{aligned}\right\} \; m = 1, 2, 3$

provided $\alpha_n + \beta_n = 0$

n roots $\varkappa^2$! Physical and nonphysical

In particular for $j = -1/2$

$(\alpha_n + \beta_n)(v=n, j=-1/2, \delta) = -(\alpha_n + \beta_n)(v=n, j=-1/2, -\delta - 1/2)$

Intersections on baselines are degenerate

$\delta = -1/4 \rightarrow \Delta = 0 \rightarrow$ all Energies on baselines !

The eigenvalues

$$w_n = \frac{\beta_n}{d_n}$$

$$W_n^{(1)} = \frac{\left\{ w_n + \frac{M_{11}(n+1,n)}{M_{12}(n+1,n)} \right\} M_{12}(n+1,n) \; \mathrm{Tr}\, M(n+1,n)}{\mathrm{Det}\, M(n+1,n)}$$

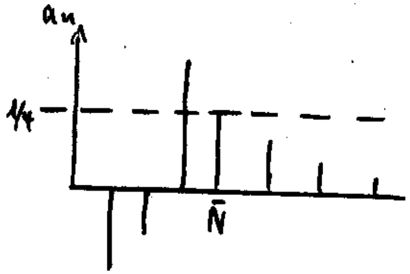
$$W_n^{(1)} = \frac{1}{1 + a_n^{(1)} W_{n+1}^{(1)}}$$

$$a_n^{(1)} = \frac{-\,\mathrm{Det}\, M(n+1,n)}{\left[\mathrm{Tr}\, M(n+1,n)\right]^2}$$

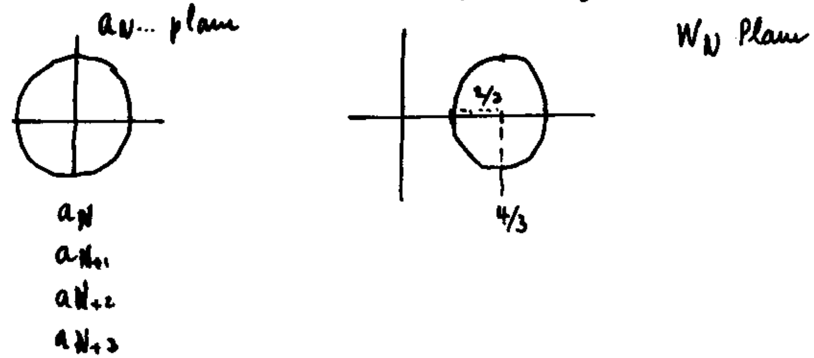
$$W_n^{(1)} = \frac{1}{1 + \frac{a_n^{(1)}}{1 + a_{n+1}^{(1)}}} = \frac{1|}{|1} + \frac{a_n^{(1)}|}{|1} + \frac{a_{n+1}^{(1)}|}{|1} + \frac{a_{n+2}^{(1)}|}{|1}$$

How to choose n conveniently?

$$\lim a_n^{(1)} \sim O(n^{-2})$$



Worpitzky (1865): First convergence theorem on Continued Fractions

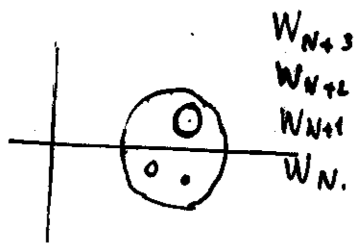


$$W_N^{(1)} = \frac{1}{1 + a_N^{(1)} W_{N+1}^{(1)}}$$

$$W_{N+1}^{(1)} = \frac{1}{1 + a_{N+1}^{(1)} \cdot W_{N+2}^{(1)}}$$

$$W_{N+m-1}^{(1)} = \frac{1}{1 + a_{N+m+1}^{(1)} \; W_{N+m}^{(1)}}$$

$$W_{N+m} = \frac{1|}{|1} + \frac{a_{N+m}|}{|1} + \frac{a_{N+m+1}|}{|1} + \cdots$$



$$W_N^{(m)} = \frac{1}{1 + a_N^{(m)} \, W_{N+m}^{(m)}}$$

Fixed point of Moebius transformation inside Worpitzky circle :

$$W_N^{(m)} = -\frac{1}{2a_N^{(m)}}\left(1-\sqrt{1+4a_N^{(m)}}\right)$$

$$\left\{\frac{\beta_N}{\alpha_N} + \frac{M_{11}(N+m,N)}{M_{12}(N+m,N)}\right\}\frac{M_{12}(N+m)\,\mathrm{Tr}\,M(N+m,N)}{\mathrm{Det}\,M(N+m,N)} = -\frac{1}{2a_N^{(m)}}\left(1-\sqrt{1+4a_N^{(m)}}\right)$$

$$\left\{\alpha_N M_{11} + \beta_N M_{12}(N+m,N)\right\} = -\alpha_N \frac{\mathrm{Det}\,M(N+m,N)}{\mathrm{Tr}\,M(N+m,N)}\frac{1}{2a_N^{(m)}}\left(1-\sqrt{1+4a_N^{(m)}}\right)$$

$$= +\alpha_N \,\mathrm{Tr}\,M(N+m,N)\left(1-\sqrt{1+4a_N^{(m)}}\right)$$

$$= \alpha_N\left\{\tfrac{1}{2}\mathrm{Tr}\,M(N+m,N) - \sqrt{\tfrac{1}{4}\mathrm{Tr}^2 M(N+m,N) - \mathrm{Det}\,M(N+m)}\right\}$$

$$\boxed{\alpha_N(M_{11} - \Lambda_2) + \beta_N M_{12}(N+m,N) = 0}$$

Sol^s on baselines as special cases!

Interpretation: Consider the eigenvalue problem

$$\begin{pmatrix}\alpha_{N+m}\\ \beta_{N+m}\end{pmatrix} = \Lambda_2\begin{pmatrix}\alpha_N\\ \beta_N\end{pmatrix} = \begin{pmatrix}M_{11}(N+m,N) & M_{12}(N+m,N)\\ M_{21}(N+m,N) & M_{22}(N+m,N)\end{pmatrix}\begin{pmatrix}\alpha_N\\ \beta_N\end{pmatrix}$$

on baseline

$$\Lambda_2 = \tfrac{1}{2}\mathrm{Tr}\,M(N+m,N) - \sqrt{\tfrac{1}{4}\mathrm{Tr}^2 M(N+m,N) - \mathrm{Det}\,M}$$