Small polaron model in atomic limit | ЖЭТФ 60, 1127 (1942)

$$H = g \sum_\sigma (b^+ + b) n_\sigma - \sum_\sigma \mu_\sigma n_\sigma + \omega b^+ b$$

$$Z = \int D[\eta^*\eta] D[b^* b] \, e^{-S[\eta^*\eta, b^* b]}$$

$$S[\eta^*\eta, b^* b] = \int_0^\beta d\tau \Big(\sum_\sigma \eta_\sigma^* \partial_\tau \eta_\sigma + b^* \partial_\tau b + g \sum_\sigma (b^* + b) \eta_\sigma^* \eta_\sigma - \sum_\sigma \mu_\sigma \eta_\sigma^* \eta_\sigma + \omega b^* b \Big)$$

phonons + electrons

$\Downarrow$

polaron

quadratic

we separate integrals $\int D[\eta_\uparrow^* \eta_\uparrow]$ and $\int D[\eta_\downarrow^* \eta_\downarrow]$

$$Z = \int D[b^* b] \, e^{-\int_0^\beta d\tau (b^* \partial_\tau b + \omega b^* b)} \cdot \int D[\eta_\uparrow^* \eta_\uparrow] \, e^{-\int_0^\beta d\tau \, \eta_\uparrow^* (\partial_\tau + g(b^* + b) - \mu_\uparrow) \eta_\uparrow} \cdot \int D[\eta_\downarrow^* \eta_\downarrow] \, e^{-\int_0^\beta d\tau \, \eta_\downarrow^* (\partial_\tau + g(b^* + b) - \mu_\downarrow) \eta_\downarrow}$$

Integrating out Grassmann variables

$$Z_\sigma = \int D[\eta_\sigma^* \eta_\sigma] \, e^{-\int_0^\beta d\tau \, \eta_\sigma^* (\partial_\tau - \mu_\sigma + g(b^* + b))} = \Big(1 + e^{\beta \mu_\sigma - \int_0^\beta d\tau \, g(b^* + b)} \Big)$$

Hence,

$$Z = \int D[b^* b] \, e^{-\int_0^\beta d\tau (b^* \partial_\tau b + \omega b^* b)} \cdot \Big(1 + e^{\beta \mu_\uparrow - \int_0^\beta d\tau \, g(b^* + b)} \Big) \cdot \Big(1 + e^{\beta \mu_\downarrow - \int_0^\beta d\tau \, g(b^* + b)} \Big)$$

Assume no external magnetic field

$$\mu_\uparrow = \mu_\downarrow = \mu$$

$$Z = \int D[b^\dagger b]\, e^{-\int_0^\beta d\tau (b^\dagger \partial_\tau b + \omega b^\dagger b)} \cdot \left(1 + e^{\beta\mu - \int_0^\beta d\tau\, \varphi (b^\dagger + b)}\right)^2 =$$

$$= \int D[b^\dagger b]\, e^{-\int_0^\beta d\tau\, b^\dagger (\partial_\tau + \omega) b} \cdot \left(1 + 2 e^{\beta\mu - \int_0^\beta d\tau\, \varphi (b^\dagger + b)} + e^{2\beta\mu - 2\int_0^\beta d\tau\, \varphi (b^\dagger + b)}\right) =$$

$$\phi(\tau) = \frac{1}{\sqrt{\beta}} \sum_n e^{i\omega_n \tau} b_n$$

$$\delta_{nm} = \frac{1}{\beta} \int_0^\beta e^{i(\omega_n - \omega_m)\tau}$$

$$= Z_1 + Z_2 + Z_3$$

$$Z_1 = \int D[b^\dagger b]\, e^{-\int_0^\beta d\tau\, b^\dagger (\partial_\tau + \omega) b} = \frac{1}{\mathrm{Det}(\partial_\tau + \omega)} =$$

$$\omega_n = \frac{2n\pi}{\beta}$$

$$= \prod_{\omega_n} \frac{1}{\beta(i\omega_n + \omega)} = \boxed{\frac{1}{1 - e^{-\beta\omega}} = Z_1}$$

$$Z_2 = 2 e^{\beta\mu} \int D[b^\dagger b]\, e^{-\int_0^\beta d\tau \left(b^\dagger (\partial_\tau + \omega) b + \varphi (b^\dagger + b)\right)} =$$

$$= 2 e^{\beta\mu} \int D[b_n^\dagger b_n]\, e^{-\sum_{\omega_n} \left(b_n^\dagger (i\omega_n + \omega) b_n + \sqrt{\beta}\varphi (b_n^\dagger + b_n)\right)}$$

<u>shift - canonical transformation</u>

$$\begin{cases} b_n = b_n - \gamma_n \\ b_n^\dagger = b_n^\dagger - \gamma_n \end{cases}$$

$$\sum_{\omega_n} b_n^+ (i\omega_n + \omega) b_n + \sqrt{\beta} g (b_n^+ + b_n)$$

$$b_n = \tilde{b}_n - \gamma_n$$
$$b_n^+ = \tilde{b}_n^+ - \gamma_n^+$$

$$(\tilde{b}_n^+ - \gamma_n^+)(i\omega_n + \omega)(\tilde{b}_n - \gamma_n) +$$
$$+ g(\tilde{b}_n^+ - \gamma_n^+ + \tilde{b}_n - \gamma_n) =$$

$$= \tilde{b}_n^+ (i\omega_n + \omega)\tilde{b}_n - \underline{\gamma_n^+ (i\omega_n + \omega)\tilde{b}_n} -$$
$$- \underline{\gamma_n (i\omega_n + \omega)\tilde{b}_n^+} + (i\omega_n + \omega)\gamma_n^+ \gamma_n +$$
$$+ g(\underline{\tilde{b}_n^+} - \gamma_n^+ + \underline{\tilde{b}_n} - \gamma_n)$$

$$(-\gamma_n^+ (i\omega_n + \omega) + \sqrt{\beta} g)\tilde{b}_n = 0 \quad \to \quad \gamma_n^+ = \frac{g\sqrt{\beta}}{i\omega_n + \omega}$$

$$(-\gamma_n (i\omega_n + \omega) + \sqrt{\beta} g)\tilde{b}_n^+ = 0 \quad \to \quad \gamma_n = \frac{g\sqrt{\beta}}{i\omega_n + \omega}$$

$$\sum_{\omega_n} \tilde{b}_n^+ (i\omega_n + \omega)\tilde{b}_n + \cancel{(i\omega_n + \omega)} \frac{g^2 \beta}{(i\omega_n + \omega)^{\cancel{2}}} -$$
$$- g \frac{2 g \beta}{i\omega_n + \omega} =$$

$$= \sum_{\omega_n} \tilde{b}_n^+ (i\omega_n + \omega)\tilde{b}_n - \sum_{\omega_n} \frac{g^2 \beta}{i\omega_n + \omega}$$

$$Z_2 = 2 e^{\beta\mu} \frac{1}{1 - e^{-\beta\omega}} e^{+\sum_{\omega_n} \frac{g^2 \beta}{i\omega_n + \omega}} =$$

$$\sum_{\omega_n} \frac{1}{i\omega_n + \omega} = -\frac{\beta}{e^{-\beta\omega} - 1}$$

$$\boxed{Z_2 = 2 e^{\beta\mu} \frac{1}{1 - e^{-\beta\omega}} e^{-g^2 \frac{\beta^2}{e^{-\beta\omega} - 1}}}$$

$$Z_3 = \int D[b^* b]\, e^{-\int_0^\beta d\tau\, b^*(\partial_\tau + \omega) b + 2\rho(b^* + b)} \cdot e^{2\beta\mu}$$

$$\{\rho \leftrightarrow 2\rho\} = e^{2\beta\mu} \frac{1}{1 - e^{-\beta\omega}}\, e^{-4\rho^2 \frac{\beta^2}{e^{\beta\omega} - 1}}$$

<u>Summary</u>

$$\boxed{Z = \underbrace{\frac{1}{1 - e^{-\beta\omega}}}_{\text{phonons}} \Big(\underbrace{1}_{\text{no electrons}} + \underbrace{2 e^{\beta\mu}\, e^{-\frac{\rho^2\beta^2}{e^{\beta\omega}-1}}}_{\text{polaron}} + \underbrace{e^{2\beta\mu}\, e^{-\frac{4\rho^2\beta^2}{e^{\beta\omega}-1}}}_{\text{polaron}} \Big)}$$

phonons

no electrons

one electron $\uparrow$ or $\downarrow$ dressed in phonons

2 electrons $\uparrow\downarrow$ dressed in phonons

polaron

polaron

In $\beta \to 0$ limit (high temperature)

$$-\frac{\rho^2\beta^2}{e^{-\beta\omega} - 1} = -\frac{\rho^2\beta^2}{1 - \beta\omega - 1} = \frac{\rho^2\beta}{\omega}$$

$$\boxed{Z = \frac{1}{1 - e^{-\beta\omega}} \left(1 + 2 e^{\beta\mu} e^{\rho^2/\omega\, \beta} + e^{2\beta\mu} e^{4 \rho^2/\omega\, \beta} \right)}$$

AJP result