31. listopada 2013.

1 Gustoća stanja

1.1 Sedlena točka u TB modelu

Energija u TB modelu:

$$E(\vec{k}) = -2t(\cos(kx_a) + \cos(k_y a) + \cos(k_z a))$$

Sedlena točka je oko energije E= -2t. Postoji 6 točaka u Brillouinovoj zoni koje odgovaraju sedlenoj točci. Usredotočiti ćemo se samo na jednu od njih:

$$\begin{aligned} |k_x| &\ll \frac{\pi}{a} \\ |k_y| &\ll \frac{\pi}{a} \\ k_z &\approx \pi - \delta k_z, \qquad \delta k_z \ll \frac{\pi}{a} \end{aligned}$$

Tada je:

$$E(\vec{k}) \approx -2t + ta^2(k_x^2 + k_y^2) - ta^2 \delta k_z^2$$

Doprinos te točke gustoći stanja:

$$\begin{aligned} \delta g(E) &= 2\frac{V}{(2\pi)^3} \int dk_x dk_y dk_z \; \delta(E + 2t - ta^2(k_x^2 + k_y^2) + ta^2 \delta k_z^2) \\ &= 2\frac{V}{(2\pi)^3 ta^3} \int dx dy dz \; \delta(\epsilon - x^2 - y^2 + z^2) \end{aligned}$$

gdje je

$$\epsilon = \frac{E + 2t}{t}$$

ϵ može biti pozitivno i negativno. To su dvije situacije koje se trebaju posebno razmotriti. Područje integracije po valnim brojevima treba ograničiti da bude u bluzini sedlenih točaka u Brillouinovoj zoni. To se može postići, npr. s ovim ograničenjem:

$$x^2 + y^2 + z^2 < 1$$

To znači da se integrira po valnim brojevima unutar sfere radijusa 1 oko sedlene točke. Uvođenje polarnih koordinata:

$$\begin{aligned} x &= \rho \cos\phi \\ y &= \rho \sin\phi \end{aligned}$$

dobivamo:

$$\delta g(E) = 2\frac{V}{(2\pi)^2 ta^3} \int d\rho dz \; \rho \, \delta(\epsilon - \rho^2 + z^2)$$

Nadalje može se uvesti slijedeća smjena varijabli:

$$\begin{aligned} \rho &= r\cosh\alpha \\ z &= r\sinh\alpha \end{aligned}$$

ako je $\epsilon > 0$, odnosno:

$$\begin{aligned} \rho &= r\sinh\alpha \\ z &= r\cosh\alpha \end{aligned}$$

ako je $\epsilon < 0$. To implicira da je:

$$r^2(\cosh^2\alpha + \sinh^2\alpha) = r^2\cosh 2\alpha < 1$$

Gornja granica područja integracije po varijabli α:

$$\begin{aligned} r^2\cosh 2\alpha_{max} &= 1 \qquad \Rightarrow \\ \alpha_{max} &= 0.5\,\mathrm{arch}\left(\frac{1}{r^2}\right) \\ &= 0.5\,\ln\left(\frac{1}{r^2} + \sqrt{\frac{1}{r^4} - 1}\right) \approx 0.5\,\ln\frac{2}{r^2} = \ln\frac{\sqrt{2}}{r} \end{aligned}$$

Očekujemo da je r^2 malo, reda veličine ϵ. U slučaju kada je $\epsilon > 0$:

$$\begin{aligned} \delta g(E) &= 2\frac{V}{(2\pi)^2ta^3}\int dr d\alpha\; r\; r\cosh\alpha\;\delta(\epsilon - r^2) \\ &= 2\frac{V}{(2\pi)^2ta^3}\int dr\; r^2\;\delta(\epsilon - r^2)\int_0^{\alpha_{max}} d\alpha\cosh\alpha = 2\frac{V}{(2\pi)^2ta^3}\int dr\; r^2\;\delta(\epsilon - r^2)\;\underbrace{\sinh\alpha_{max}}_{\approx 0.5\frac{\sqrt{2}}{r}} \\ &= \frac{V}{(2\pi)^2ta^3}\int dr\; r^2\;\delta(\epsilon - r^2)\;\frac{\sqrt{2}}{r} = \frac{V}{\sqrt{2}(2\pi)^2ta^3} = \text{konst.} \end{aligned}$$

ako je $\epsilon < 0$:

$$\begin{aligned} \delta g(E) &= 2\frac{V}{(2\pi)^2ta^3}\int dr d\alpha\; r\; r\sinh\alpha\;\delta(-|\epsilon| + r^2) \\ &= 2\frac{V}{(2\pi)^2ta^3}\int dr\; r^2\delta(r^2 - |\epsilon|)\int_0^{\alpha_{max}} d\alpha\sinh\alpha \\ &= 2\frac{V}{(2\pi)^2ta^3}\int dr\; r^2\delta(r^2 - |\epsilon|)\left(\underbrace{\cosh\alpha_{max}}_{\approx 0.5\frac{\sqrt{2}}{r}} - 1.0\right) \\ &= \frac{V}{\sqrt{2}(2\pi)^2ta^3}\int de\;(1 - \sqrt{2e})\;\delta(e - \epsilon) \\ &= \frac{V}{\sqrt{2}(2\pi)^2ta^3}\;\left(1 - \sqrt{2|\epsilon|}\right) \end{aligned}$$

2 Gustoća stanja 2d TB modelu

Energija u TB modelu:

$$
\begin{aligned}
E(\vec{k}) &= -2t\left[\cos(k_x a) + \cos(k_y a)\right] \\
&= -4t + 2t\left[1 - \cos(k_x a) + 1 - \cos(k_y a)\right] \\
&= -4t + 4t\left[\sin^2\left(\frac{k_x a}{2}\right) + \sin^2\left(\frac{k_y a}{2}\right)\right]
\end{aligned}
$$

Uvodimo nove varijable r i ϕ:

$$
\begin{aligned}
\sin\left(\frac{k_x a}{2}\right) &= r\,\cos\left(\frac{\phi}{2}\right) \qquad \Rightarrow \qquad k_x = \frac{2}{a}\arcsin\left(r\,\cos\left(\frac{\phi}{2}\right)\right) \\
\sin\left(\frac{k_y a}{2}\right) &= r\,\sin\left(\frac{\phi}{2}\right) \qquad \Rightarrow \qquad k_x = \frac{2}{a}\arcsin\left(r\,\sin\left(\frac{\phi}{2}\right)\right)
\end{aligned}
$$

Jakobijan:

$$
\begin{aligned}
\left|\frac{\partial(k_x, k_y)}{\partial(r,\phi)}\right| &= \begin{vmatrix} \dfrac{2\,\cos\left(\frac{\phi}{2}\right)}{a\sqrt{1 - r^2\cos^2\left(\frac{\phi}{2}\right)}} & -\dfrac{r\,\sin\left(\frac{\phi}{2}\right)}{a\sqrt{1 - r^2\cos^2\left(\frac{\phi}{2}\right)}} \\ \dfrac{2\,\sin\left(\frac{\phi}{2}\right)}{a\sqrt{1 - r^2\sin^2\left(\frac{\phi}{2}\right)}} & \dfrac{r\,\cos\left(\frac{\phi}{2}\right)}{a\sqrt{1 - r^2\sin^2\left(\frac{\phi}{2}\right)}} \end{vmatrix} \\
&= \frac{2r}{a^2\sqrt{1 - r^2\cos^2\left(\frac{\phi}{2}\right)}\sqrt{1 - r^2\sin^2\left(\frac{\phi}{2}\right)}} = \frac{2r}{a^2\sqrt{1 - r^2 + r^4\cos^2\left(\frac{\phi}{2}\right)\sin^2\left(\frac{\phi}{2}\right)}} \\
&= \frac{2r}{a^2\sqrt{1 - r^2 + 0.25r^4\sin^2\phi}} = \frac{2r}{a^2\sqrt{(1 - r^2 + 0.25r^4) - 0.25r^4\cos^2\phi}} \\
&= \frac{2r}{a^2\sqrt{1 - r^2 + 0.25r^4}}\,\frac{1}{\sqrt{1 - k^2\sin^2\left(\frac{\pi}{2} - \phi\right)}}
\end{aligned}
$$

gdje je:

$$
k = \frac{0.5r^2}{\sqrt{1 - r^2 + 0.25r^4}}
$$

Gustoća stanja:

$$\begin{aligned}
g(E) &= \frac{2}{(2\pi)^2}\int dk_x dk_y\ \delta\left(E+2t\left[\cos(k_x a)+\cos(k_y a)\right]\right) \\
&= \frac{2\cdot 4}{(2\pi)^2}\int\limits_0^{\pi} dk_x \int\limits_0^{\pi} dk_y\ \delta\left(E+4t-4tr^2\right) = \frac{2}{\pi^2}\int\limits_0^{1} dr \int\limits_0^{\pi} d\phi\ \left|\frac{\partial(k_x,k_y)}{\partial(r,\phi)}\right|\ \delta\left(E+4t-4tr^2\right) \\
&= \frac{2}{\pi^2}\int\limits_0^{1} dr \int\limits_0^{\pi} d\phi\ \delta\left(E+4t-4tr^2\right) \frac{2r}{a^2\sqrt{1-r^2+0.25r^4}}\ \frac{1}{\sqrt{1-k^2\sin^2\left(\frac{\pi}{2}-\phi\right)}} \\
&= \frac{4}{\pi^2}\int\limits_0^{1} dr\delta\left(E+4t-4tr^2\right) \frac{2r}{a^2\sqrt{1-r^2+0.25r^4}}\ \int\limits_0^{0.5\pi} d\phi'\ \frac{1}{\sqrt{1-k^2\sin^2\phi'}} \\
&= \frac{4}{\pi^2}\int\limits_0^{1} dr\delta\left(E+4t-4tr^2\right) \frac{2r}{a^2\sqrt{1-r^2+0.25r^4}}\ F(k) \\
&= \frac{1}{(a\pi)^2 t}\frac{F(k_E)}{\sqrt{1-r_E^2+0.25r_E^4}}
\end{aligned}$$

gdje je:

$$\begin{aligned}
r_E &= \sqrt{1-\frac{|E|}{4t}} \\
k_E &= \frac{0.5r_E^2}{\sqrt{1-r_E^2+0.25r_E^4}}
\end{aligned}$$