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Effective Spin Hamiltonian

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ABSTRACT In the introduction, definition of Hamiltonian (Relativistic & Non-Relativistic), Euler's equation and Schrodinger's time dependent equation are used. Hamiltonian field theory (given by Pruskin) is used Anderson Model and Jacobian Transformation are applied. Perturbation and Green function are used. Dimmock Hamiltonian, Dugaev and Litvinov spins (S_1 and S_2) are used. Heff. in $P_{b_{1-x}}M_{n_x}A\left(A = T_e, S_e, S\right)$ is obtained. Various temperature and band parameters for $P_{b_{1-x}}M_{n_x}T_e$ for x = 0.1 & x = 0.01 are listed in table.

KEYWORDS Euler's equation, Schrodinger's time dependent equation, Pruisken field theory, Anderson Model, Jacobian Transformation, Perturbation & Green function, Dugaev & Litvinov spins.

INTRODUCTION

Classically; Hamiltonian function is defined as

$$H = \sum p_i \cdot \dot{q}_i - L$$

Where p is momentum & L is Lagrangian

$$\because p = \frac{\partial L}{\partial V} = \frac{m_0 v}{\left(1 - \frac{v^2}{c^2}\right)^{\frac{3}{2}}} + qA$$

$$\& \ L = \left[\frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} - 1\right] moc^2 - q\varphi + q\left(\vec{v} \cdot \vec{A}\right) \quad \text{where } \vec{A} = \text{Arbitrary}$$

$$\therefore H = \left[\frac{m_0 V}{\left(1 - \frac{v^2}{c^2}\right)^{\frac{3}{2}}} + qA\right] v - \left[\left\{\frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} - 1\right\} m_0 c^2 - q\varphi + q\left(\vec{v} \cdot \vec{A}\right)\right]$$

$$\therefore H = \frac{m_0 V^2}{\left(1-\frac{v^2}{c^2}\right)^{\frac{3}{2}}} - \left[\left\{\frac{1}{\sqrt{1-\frac{v^2}{c^2}}} - 1\right\} m_0 C^2\right] + q\varphi \text{ --------------------(1)}$$

Which is relativistic Hamiltonian in an electromagnetic field theory. For infinitesimal cells, Hamiltonian can be written as

$$H = \int \pi\left(\dot{\psi} - L\right)\delta\tau$$

$\Rightarrow H = \int H d\tau$ here H = Hamiltonian density = $\pi\dot{\psi} - L$

Hamilton's variational principle[8] is given by

$$\delta\int_{t_1}^{t_2} L \cdot dt = 0;\ \delta q_i(t_1) = \delta q_i(t_2) = 0$$

$$\therefore \delta\int_{t_1}^{t_2} L \cdot dt = \delta\int_{t_1}^{t_2}\int L\left(\psi, \nabla\psi; \dot{\psi}, t\right) dt\ d\tau = 0$$

Where $L = \int L\left(\psi, \nabla\psi, \dot{\psi}, t\right) d\tau$

$$\Rightarrow \int_{t_1}^{t_2}\iiint\left[\frac{\partial L}{\partial\psi}\delta\psi + \sum_{k=1}^{3}\frac{\partial L}{\partial\psi/\partial x_k}\frac{\partial}{\partial x_k}(\delta\psi) + \frac{\partial L}{\partial\dot{\psi}}\frac{\partial}{\partial t}(\partial\psi)\right] dt\ dx_1 dx_2 dx_3 = 0$$

Where $d\tau = dx_1 dx_2 dx_3$

$$\Rightarrow \int_{t_1}^{t_2}\iiint\left[\frac{\partial L}{\partial\psi} - \sum_{k=1}^{3}\frac{\partial}{\partial x_k}\left\{\frac{\partial L}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)}\right\} - \frac{\partial}{\partial t}\cdot\frac{\partial L}{\partial\dot{\psi}}\right]\delta\psi dt\ dx_1 dx_2 dx_3 = 0$$

Since $\delta\psi$'s are arbitrary, so above equation is equivalent to the differential equation

$$\frac{\partial L}{\partial\psi} - \sum_{k=1}^{3}\frac{\partial}{\partial x_k}\left\{\frac{\partial L}{\partial\left(\frac{\partial\psi}{\partial x_k}\right)}\right\} - \frac{\partial}{\partial t}\left(\frac{\partial L}{\partial\dot{\psi}}\right) = 0$$

This classical field equation is called Euler's equation. Now Schrodinger's time dependent Equation is $H\psi = E\psi$ -------------- (2)

which gives motion of non-relativistic material particle.

Here $H = \frac{p^2}{2m} + v(r) = \frac{-\hbar^2}{2m}\nabla^2 + v(r)$ is called Hamiltonian operator.

$E = i\hbar\frac{\partial}{\partial t}$ is called energy operator.

V(r) is real & E_k are also real.

The eigen value of Hamiltonian operator can be written as

$$H_{op}\psi = E\psi \text{ --------------- (3)}$$

Where E is the eigen value of H_{op} & represents energy of the system. ψ is the eigen function of H_{op}. The eigen value E must be purely real otherwise ψ would be divergent either at $x = \infty$ or at $x = -\infty$. The eigen function of H_{op} are states for which the total energy of the system has a definite value.

The Hamiltonian field theory was given by Pruisken in 1984, first. The original formula is

$$|\nabla Vs| << \frac{\hbar\omega_c}{\rho}. \qquad \text{--------------------- (4)}$$

The Hamiltonian Q fields is given by change of variables[1]

$$Q(r) \to T^{-1}(r)P(r)T(r)$$

Where $T(r) = U(2m); T(r) =$ critical field component and $P(r)=P^{+}(r) \equiv p_{ab}^{p7}(r)$ is block diagonal in the P-indices. This result will serve as the basic starting point for the effective field theory. Anderson model is introduced in it & in terms of the new field variables[2] the equation can be written as

$$Z = \int D(T) \int D(P) I(P) e^{G[P,T]} \qquad \text{----------------------- (5)}$$

Where I(P) is Jacobian transformation and $I(P) =_i \pi_j \left[\lambda_t^1 - \lambda_j^2\right]^2$

The zeroth order theory exhibits diamagnetic[5] edge currents and hence long range behavior along the perimeter of the system.

For effective Hamiltonian field theory are bare parameters[3]
$\sigma_{xx} = 0$ and σ_{xy} = integer are used.

$$\left.\begin{array}{l} \sigma_{xx} = \sigma_{xx}^{o} + C_0 + \sum_{n=1}^{\infty} C_n \cos\left(2\pi n\, \sigma_{xx}^{o}\right) \\ \sigma_{xy} = \sigma_{xy}^{o} + \sum_{n=1}^{\infty} \theta_n \sin\left(2\pi n\, \sigma_{xy}^{o}\right) \end{array}\right] - \qquad \text{----------------------- (6)}$$

These are entirely topological in origin & unobservable in the asymptotic perturbative series in $1/\sigma_{xx}^{o}$

Clearly on the series $\sigma_{xy}^{o} = \text{integer}$. The theory is invarient under the swift

$$\sigma_{xy}^{o} \to \sigma_{xy}^{o} + \text{integer}$$

Hence, σ_{xy}^{o} slightly deviating from integer values. The fixed point can be associated with a delocalisation of the electronic wave functions. One expect a singular part in the free energy per unit area which scales is

$$\tau_s\left(\tilde{\theta}, \tilde{\sigma}\right) = b^{-2}\, \tau_s\left(b^{y}\tilde{\theta}, b^{-y}\tilde{\sigma}\right), y, \tilde{y} > 0 \qquad \text{---- -------------- (7)}$$

Where $\tilde{\theta}$ and $\tilde{\sigma}$ represent linear deviations from the fixed point values σ_{xy}^{*} and σ_{xx}^{*} respectively.
Hence localisation length given as

$$\xi\left(\tilde{\theta}, \tilde{\sigma}\right) = b\xi\left(b^{y}\tilde{\theta}, b^{\overset{\sim}{-y}}\tilde{\sigma}\right) \qquad \text{------------------ (8)}$$

Schrodinger equation with eigen function is applied

$$\psi(r,t) = \sum_k c_k \psi_k(r) e^{-i}\xi_k t / \hbar \qquad \text{------------------- (9)}$$

Where $c_k = \int d^3{}_r \psi_k{}^* (r) \psi_k (r,0)$

Green function is used in the field theory

$\psi(r,t) = \int d^3{}_r \psi(r,t) \psi^* (r',0) \psi(r',0)$

$= \int d^3{}_r k(r,r',t) \psi(r,0)$ -------------------(10)

Here, $k(r,r',t) = \psi(r,t) \psi^* (r,0)$

The time variation is introduced through the Hamiltonian operator as,

$\psi(r,t) = e^{iHt/\hbar} \psi(r) \ell^{-iHt/\hbar}$ -------------------(11)

Thus, the green's function provides information on the propagation of excitation as given in equation (X). It is held when returning the system to the ground state. It is respond to the total Hamiltonian. Generally, the electron-phonon[6] interaction gives perturbation theory in lowest order.

The Hamiltonian is usually written in terms of

$H = H_0 + V$ ------------------ (12)

Where H_o contains only those terms for which the Schrodinger equation can be solved exactly and V_0 contains these terms for which the perturbation approach is necessary.

Considering the operator,

$U(t) = e^{-itHo/\hbar} e^{-itH/\hbar}$ ------------------(13)

$\therefore dU(t) = e^{iH_o t/\hbar} (i/\hbar)(H_o - H) e^{-iHt/\hbar}$

$= e^{iH_o t/\hbar} (i/\hbar)(-v) e^{-(ih_o t/\hbar)} e^{-iHt/\hbar}$

$= -(i/h) v(t) U(t)$ -------------------(14)

Where $v(t) = e^{iH_o t/\hbar} V e^{-iH_o t/\hbar}$

Here H_o governs time dependence of the operator while the perturbation provides a slow variation of resulting states. So equation (xiv) can be solved as

$U(t) = 1 - (i/\hbar) \int_0^t dt' V(t') U(t')$ ------------------(15)

Which is an integral equation for U(t)

This equation yields the perturbation series

$$U(t) = \sum_{n=0}^{\infty} (-i/\hbar)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots\ldots\ldots\ldots \int_0^{tn-1} dt_n v(t_1) \ldots\ldots\ldots v(t_n)$$

$= \tilde{T} \exp\left[-i/\hbar \int_0^t dt' V(t') \right]$ -------------------(16)

Here $\tilde{T}$ be the time ordering operator which is an increasing function as one moves from the right to left. U(t) is used in evaluating Green's function in term of total Hamiltonian H.

$G^< (r,t;r',t') = \mp i < e^{iHt^1/\hbar} \psi^+ (r') e^{iH(t'-t')/\hbar} \quad \psi(r) e^{-iHt/\hbar} >$

$= \mp i < U^+ (t') \psi_0^+ (r',t') U(t') U^+ (t) \psi_0 (r,t) U(t)$ -------- (17)

Where subscript on the field operator indicates that the time evolution is only with H_o. The effective spin Hamiltorian in $P_{b_{1-x}} M_{n_x} A(A = Te, Se, S)$ has been obtained as a result of indirect exchange between M_n atoms via electrons and holes. It is calculated for non zero temperature using Green function. The band Hamiltonian H_o is well approximated by a two and Dimmock Hamiltonian[4].

i.e., $H_0 = V_x \hat{\alpha}_x p_x + V_y \hat{\alpha}_y p_y + v_2 \hat{\alpha}_z p_z + B/2 . E_g$ ------- (18)

where $\hat{\alpha} = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, B = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$

σ is the Pauli matrices vector. I is a two dimensional unit matrix. V is the velocity matrix element & E_g is the energy gap.

In this work, Dugaev and Litvinov obtained with spins S_1 & S_2,

$$H_{eff} = J^2T / \left((2\pi\hbar)^6 N^2 \right) \sum_{\omega_n} \left\{ S_1S_2 \left[-\omega_n^2 I_1 + \left(Eg^2/4 \right) I_1 - \left(V^2/R^2 \right) I_3 \right] \right\} + \left(2V^2/R^4 \right) I_3 (S_1R)(S_2R) \quad \text{------ (19)}$$

At t = 0, above equation can be written as

$$H_{eff} = J^2T / \Big(16(\pi NR)^2 (\hbar v)^4 \cdot - \sum_{\omega_n} 2\left(\partial^2 / \partial b^2 \right) - (4/b)\left(\frac{\partial}{\partial b} \right)$$

$$+ \left(4/b^2 \right) - \left(E_g{}^2/2 \right) \exp\left(-b\sqrt{\ } \omega_n^2 + E_g{}^2/4 \right) \Big) S_1S_2$$

$$+2\sum_{\omega_n} \left[\left(\frac{\partial^2}{\partial b^2} \right) - \left({}^{4}\!/_{b} \right)\left({}^{\partial}\!/_{\partial b} \right) + \left({}^{4}\!/_{b}{}^{2} \right) \right] \exp\left(-b\sqrt{\ } \left(\omega_n^2 \right) + E_g{}^2/4 \right) \cdot \frac{(S_1R)\cdot(S_2R)}{R^2} \quad \text{----------(20)}$$

RESULT AND DISCUSSION

The effective spin Hamiltonian is expressed as a sum of a linear combination of first and second derivatives of $\exp\left(-b\sqrt{\ } \left(\omega_n^2 + Eg^2/4 \right) \right)$. Equation (20) converges so alternating order of summation and differentiating the effecting spin Hailtonian takes the form,

$$H_{eff} = C\left[-\left\{ \left(2{}^{\partial^2}\!/_{\partial b^2} \right) - (4/b)(\partial/\partial b) + \left(4/b^2 \right) - E_g{}^2/2 \right\} \right] \cdot ZS_1S_2 + \left(\left({}^{\partial^2}\!/_{\partial b^2} \right) - (4/b)\left(\frac{\partial}{\partial b} \right) + \left(4/b^2 \right) \right)$$

$$\cdot Z\left[(S_1R)(S_2R)/R^2 \right]$$

$$\therefore H_{eff} = -C\hat{D}_1 Z(S_1S_2) + 2C\hat{D}_2 Z\left[(S_1R)(S_2R)/R^2 \right] \quad \text{---------- (21)}$$

Here $Z = T\sum_{\omega_n} \exp\left(-b\sqrt{\ } \left(\omega_n^2 + E_g{}^2/4 \right) \right)$

$C = J^2 / \sum 16\pi^2 N^2 R^2 (\hbar v)^4 \ \ ]$

$\hat{D}1$ & $\hat{D}2$ are differential operators acting on Z. For T = 0 the sum Z over ω_n may be replaced by integral over $d\omega$. For non zero E_g & T, the sum Z is not analytically calculable. At room temperature (300K) the gap energy E_g must be much smaller than approximately 150 meV. For lower temperature the allowed E_g value are even smaller. In the general case of arbitrary E_g the effective spin Hamiltonian given by equation (21) can't be expressed in terms of elementary special function.

Some numerical results for various temperatures and band structure parameters for $P_{b_{1-x}} M_{n_x} Te$ and x = 0.1 & x = 0.01 are listed in table 1.

Table 1:

$E_{g(ev)}$	R A°	T (k)	**a**	ξ	$\in$	$\lvert\tau_1\rvert$	$\lvert\tau_2\rvert$	$\lvert\tau_3\rvert$	τ
0.22	8.4	300	0.78	5.46	1.3	3.5×10^{-3}	1.8×10^{-5}	1.4×10^{-7}	0.9965
0.22	12.0	300	1.11	3.82	1.3	8.1×10^{-3}	4.4×10^{-5}	3.4×10^{-7}	0.9919
0.22	18.0	300	1.67	2.55	1.3	2.2×10^{-2}	1.3×10^{-4}	1.1×10^{-6}	.09782

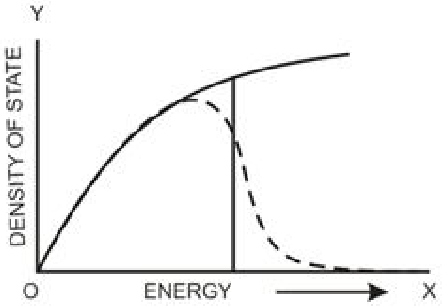

Figure 1:

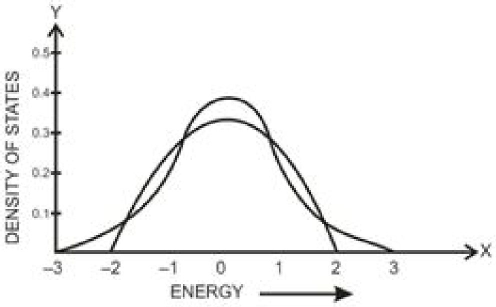

Figure 2:

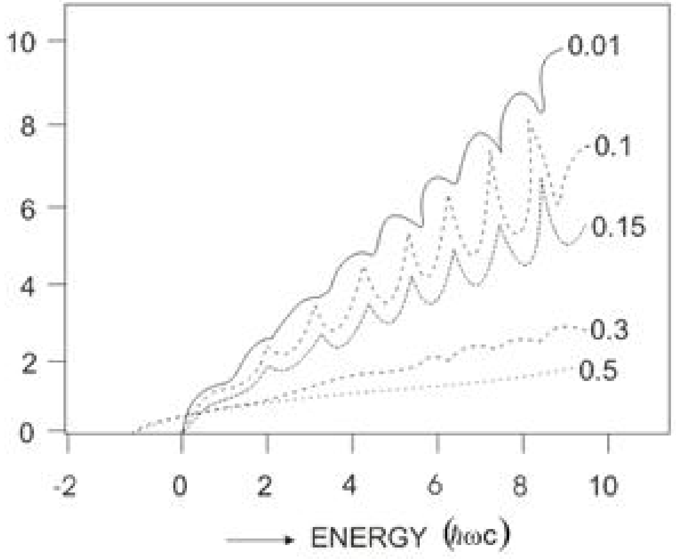

Figure 3:

CONCLUSION

At non-zero temperature, the analysis of effective spin Hamiltonian presented above points out, the zero temperature approach is quite accurate.

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